



ADA 064056

DDC FILE COPY.

COMPUTER CODE TO ANALYZE ALPHA SPECTRA USING A SPECTRAL STRIPPING APPROACH

THESIS

AFIT/GNE/PH/78D-/6

John R. Harstine Captain USAF



Approved for public release; distribution unlimited

14) AFIT/GNE/PH/78D-/6

COMPUTER CODE TO ANALYZE ALPHA
SPECTRA USING A SPECTRAL
STRIPPING APPROACH.

9 moster's THESIS,

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

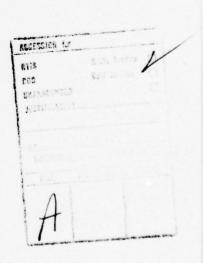
(12) 143p

John R./Harstine B.S.

Captain USAF

Graduate Nuclear Engineering

December 1978



Approved for public release; distribution unlimited

012 225

Sur

Preface

This thesis is part of a continuing study of the problem of computer analysis of alpha particle spectra. The performance of the program under ideal conditions was studied using Gaussian curves. Po²¹⁰ was used to prepare sources of different thicknesses to obtain a library of curves. These were then used to analyze samples of americium and plutonium. Using a reference peak with a full width at half maximum that matched the sample gave the most accurate analysis.

Several people contributed to the success of this thesis. Dr. George John and Dr. Richard Hagee, my thesis advisors, provided ideas, resources, and encouragement all summer. Harold Kirby and Roland Armani contributed their ideas and experience in the preparation of sources.

Dr. Dave Hardin and Captain Bruce Stinson were both helpful in my programming efforts. To them in particular, and to all of the AFIT physics laboratory and metal shop personnel as well, I extend my sincere thanks.

Finally, I would like to thank Mrs. Donna Hadley, whose typing contributed significantly to the successful completion of this thesis.

Contents

							P	age
Preface						•		ii
List of	Figures					•	•	v
List of	Tables			•	•	•	.v	111
Abstract		•			•	•	•	ix
I.	Introduction			•	•			1
	Basic Problem			:	:	:	:	1 3
	Problem Statement	•	• •	•	•	•	•	7
	Plan of Attack	•	• •	•	•	•	•	8
	Summary of Work Done Overview of Thesis		• •					9
II.	Theory						•	10
	Alpha Decay							10
	Alpha Particle Interaction							13
	Alpha Particle Detection							14
	Relation of Counts to Activity .							16
	Need for Computer Peak Analysis							17
	Computer Peak Analysis	•	• •	•	•	•	•	18
III.	Experimental Equipment and Procedur	е		•	•	•	•	20
	Introduction	•		•	•	•	•	20
	Alpha Spectroscopy Equi ment	•		•	•	•	•	20
			• •				•	20
	Detector							22 22
	Amplifiers	•	• •	•	•	•	•	22
	Multi-channel Analyzers							22
	Assay Equipment	•	• •	•	•	•	•	23
	Preparation of Sources	•	• •	•	•	•	•	23
	Kirby Method	•	• •	•	•	•	•	23
	Armani Electroplating Method .			:		:	:	24
IV.	Experimental Results							25
	Introduction							25
	Sources Prepared	:		•				25
								27
	Spectral Results		•	•		•		28

		Page
V. Pr	ogram Modifications	43
	Introduction	43 44 45
VI. Pr	rogram Computation Results	46
	Introduction Conjured Spectra Separation Effect Reference Width Effect Real Spectra 512 Channel Analyses 2048 Channel Analyses	46
VII. Co	nclusions and Recommendations	62
	Conclusions	62 63 63
Bibliograp	hy	65
Appendix A	: Utility Programs	66
Appendix B	Program SCRIPT	69
Appendix C	: User Instructions for SCRIPT	71
Appendix D	Program SPECTRE	72
Appendix E	: User Instructions for SPECTRE	78
Appendix F	Overview of Program ALFAIC	80
Appendix G	Input Cards for ALFAIC	84
Appendix H	Program ALFAIC	90
Appendix I	: Miscellaneous Plots	118
Vita		131

List of Figures

Figure	Pe	age
1	Ra DEF #15 (Unoxidized) Unbiased Run 40,000 sec	2
2	Am ²⁴¹ (ORTEC) Unbiased Run 0.6 KeV/Channel 10 Ksec	4
3	Ra DEF #11 (Unoxidized) 0.6 KeV/Channel 40,000 sec Ra DEF #13 (Unoxidized) 0.6 KeV/Channel 40,000 sec	5
4	Pu ²⁴⁰ #1 Armani 77 0.6 KeV/Channel 20,000 sec Pu ²⁴⁰ #2 Armani 77 0.6 KeV/Channel 10,000 sec	6
5	Raised and Parallel Views of Vacuum Chamber for Alpha Spectroscopy (Not to Scale)	21
6	Am ²⁴¹ ORTEC 1/21/69 0.6 KeV/Channel 10,000 sec	33
7	Pu ²⁴⁰ #2 Armani 77 0.6 KeV/Channel 10,000 sec .	34
8	Pu ²⁴⁰ #1 Armani 77 0.6 KeV/Channel 20,000 sec .	35
9	Ra DEF #10 (Oxidized) 0.6 KeV/Channel 40,000 sec	36
10	Ra DEF #11 (Oxidized) 0.6 KeV/Channel 40,000 sec	37
11	Ra DEF #12 (Oxidized) 0.6 KeV/Channel 40,000 sec	38
12	Ra DEF #13 (Oxidized) 0.6 KeV/Channel 40,000 sec	39
13	Ra DEF #14 (Oxidized) 0.6 KeV/Channel 40,000 sec	40
14	Ra DEF #15 (Oxidized) 0.6 KeV/Channel 40,000 sec	41
15	Ra DEF #16 (Oxidized) 0.6 KeV/Channel 40,000 sec	42
16	Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 1000, 10000	50
17	Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 5000, 10000	51
18	Randomized Gaussian Peaks. Separation = 20 Channels. Heights are 5000, 10000	52

Figure		P	age
19	Analysis of (σ = 20) Gaussian Peaks with Reference Peaks of Different Widths. Ratio of Peak Heights = 10:1		55
20	Analysis with Reference Peaks of Different Widths. Standard Deviation of Peaks Analyzed = 20. Ratio of Peak Heights = 10:5	•	55
21	Analysis of Pu ²⁴⁰ #1 with Various Ra DEF Samples. All Spectra from ORTEC 100 mm ² SBD at 30-35 V Net Bias		58
22	Analysis of Am ²⁴¹ with Various Ra DEF Samples. All Spectra from ORTEC 100 mm ² SBD at 30-35 V Net Bias		58
23	Results of 2048 Channel Analyses of Pu ²⁴⁰ #1 with Various Ra DEF Samples. All Spectra from ORTEC 100 mm ² SBD at 30-35 V Net Bias		61
24	ALFAIC Overall Flow Chart		81
25	Ra DEF #11 (Unoxidized) 0.6 KeV/Channel 40,000 sec		119
26	Ra DEF #12 (Unoxidized) 0.6 KeV/Channel 40,000 sec		120
27	Ra DEF #12 (Unoxidized) 0.6 KeV/Channel 40,000 sec		121
28	Ra DEF #14 (Unoxidized) 0.6 KeV/Channel 40,000 sec	•	122
29	Ra DEF #15 (Unoxidized) 0.6 KeV/Channel 40,000 sec		123
30	Ra DEF #16 (Unoxidized) 0.6 KeV/Channel 40,000 sec		124
31	Randomized Gaussian Peaks. Separation = 100 Channels. Heights are 10000, 20000		125
32	Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 10000, 20000	•	126
33	Randomized Gaussian Peaks. Separation = 100 Channels. Heights are 1000, 2000		127
34	Randomized Gaussian Peaks. Separation = 50		128

Figure								Ē	age
35	Randomized	Gaussian Peaks.	Separation	=	100	0			
	Channels.	Heights are 100,	200	•	• •	•	•	•	129
36	Randomized	Gaussian Peaks.	Separation	=	50				
	Channels.	Heights are 100,	200	•			•	•	130

List of Tables

Table	<u>Pa</u>	ige
I	Characteristics of Some Radioactive Isotopes (Data from Lederer (Ref 10))	11
11	Comparison of Full Width at Half Maximum in 2048 Channel Biased Spectra From 100 mm ² Surface Barrier Detector with Quantity Added Pb(NO ₃) ₂ in the Sample	26
III	Results of Assay of Samples 1-9 in 2π Geometry Gas Flow Proportional Counter at 1000V (α) and 1600V (α + β)	29
IV	Results of Assay of Samples 10-21 in 2π Geometry Gas Flow Proportional Counter at 1000V (α) and 1800V (α + β)	30
V	Results of Assay of Samples 10-16 in 2π Geometry Gas Flow Proportional Counter at 1000V (α) and 1800V ($\alpha + \beta$)	31
VI	Errors Versus Separation Distance for Gaussian Peaks $1/2 = 5:10$, $\sigma = 20$, Peak 1 in Channel 250, True Area ≈ 572000	47
VII	Errors Versus Separation Distance for Gaussian Peaks $1/2 = 1:10$, $\sigma = 20$, Peak 1 in Channel 250, True Area ≈ 417000	48
VIII	Analysis of $(\sigma = 20)$ Gaussian Peaks with Reference Peaks of Varying σ . Ratio of Peak Heights = $10:1$ Separation = $50(2.5 \sigma)$	53
IX	Analysis of $(\sigma = 20)$ Gaussian Peaks with Reference Peaks of Varying σ . Ratio of Peak Heights = $10:5$ Separation = $50(2.5 \sigma)$	54
x	Analysis of Plutonium and Americium with Polonium Spectra of Varying Self-Absorption. All Spectra from 100 mm ² ORTEC Surface Barrier Detector at 30-35 V Net Bias	57
XI	Results of 2048 Channel Analyses of Pu ²⁴⁰ #1	60

Abstract

Sources of Po²¹⁰ of varying thicknesses were prepared by an evaporative precipitation method. Sources of Am²⁴¹ and Pu²⁴⁰ were analyzed with the spectra of these sources as reference peak functions using a modification of an existing computer code. The results showed a reduction of the residual from using a reference peak with a full width at half maximum close to that of the analyzed source. The performance of the computer code was also studied using randomized Gaussian peaks.

COMPUTER CODE TO ANALYZE ALPHA SPECTRA USING A SPECTRAL STRIPPING APPROACH

I. Introduction

This report is part of a continuing study of alpha spectra obtained from solid state detectors. The general purpose of this study is to learn how to use these spectra to obtain a more accurate analysis of small quantities of alpha-emitting nuclides. The specific purpose of this thesis was to take a computer program which analyzes alpha spectra using a spectral stripping approach and modify it to compensate for the differences in the shape of spectra obtained from different sources.

Basic Problem

Solid state alpha spectroscopy is a technique widely used to analyze microscopic quantities of unknown substances to determine the amounts in the sample of various heavy nuclides such as plutonium. However, the accuracy of this analysis is limited by several problems inherent in alpha decay and its detection. The spectrum from particles of a single energy is spread over the range of energies from the initial energy of decay practically down to zero. This can be seen clearly in Figure 1, which is a full-range spectrum

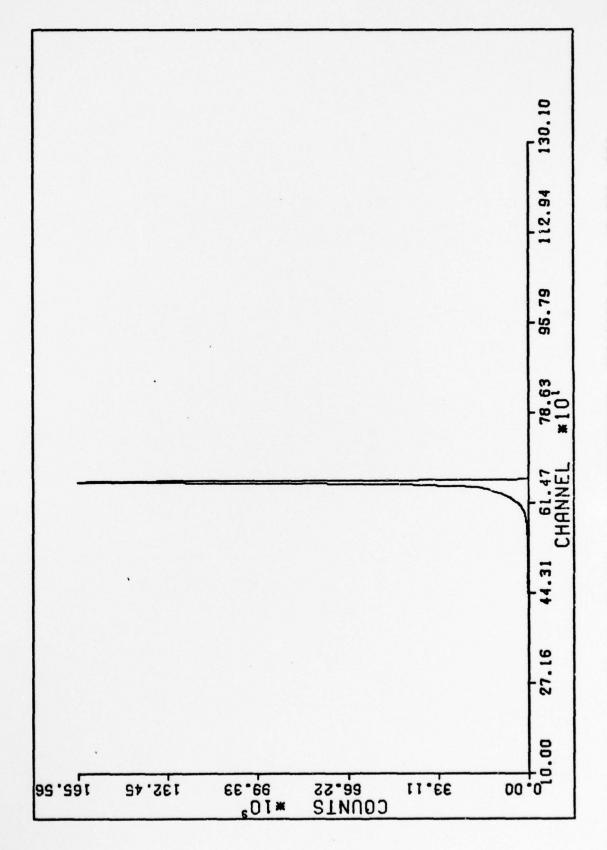


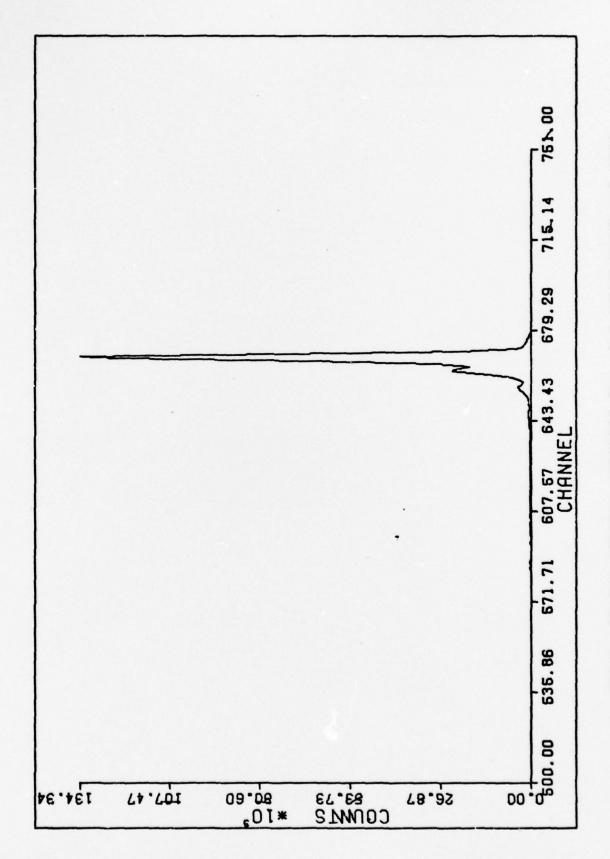
FIG 1. RR DEF # 15 (UNBXIDIZED) UNBIRSED RUN 40,000 SEC.

from a source of Radium DEF (Po²¹⁰). In addition, most alpha emitters can decay to more than one energy state in the daughter nucleus yielding alpha particles of different discrete energies in the process. The spectra from the different energies are then overlapped, as seen in Figure 2, which represents part of a spectrum from Americium 241. Finally, the shape of the curves from the individual alpha energy peaks and of the resulting combined spectra varies from sample to sample because of differences in the selfabsorption. This is shown in Figures 3 and 4, which are overlapping normalized spectra from different samples of Po²¹⁰ (Figure 3) and Pu²⁴⁰ (Figure 4).

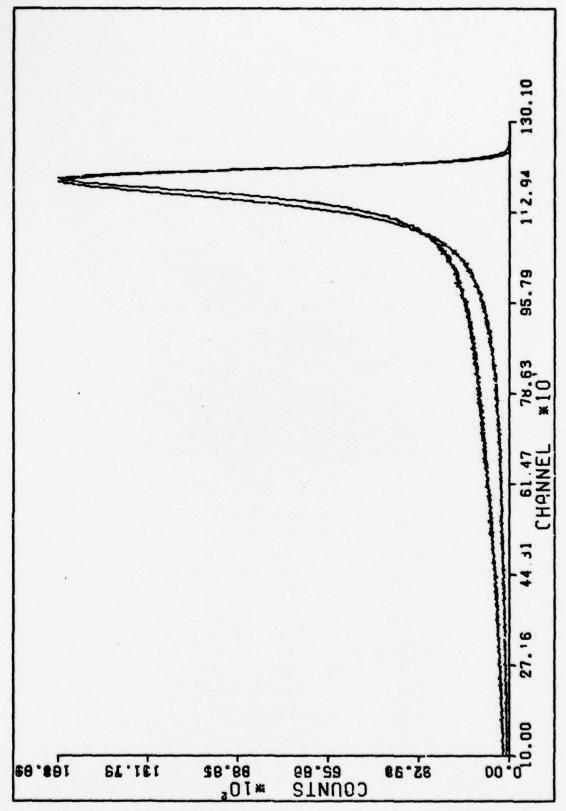
If a sample is to be analyzed accurately, the counts of a given energy must be separated into the individual components from the particles of different original energies. This requires a reference curve of the correct shape for the particular sample to be analyzed. The components of the entire energy range for each energy alpha particle are then summed. Finally, the contributions from all the alpha particles for each nuclide are summed to give the total number of decays for that particular nuclide.

Background

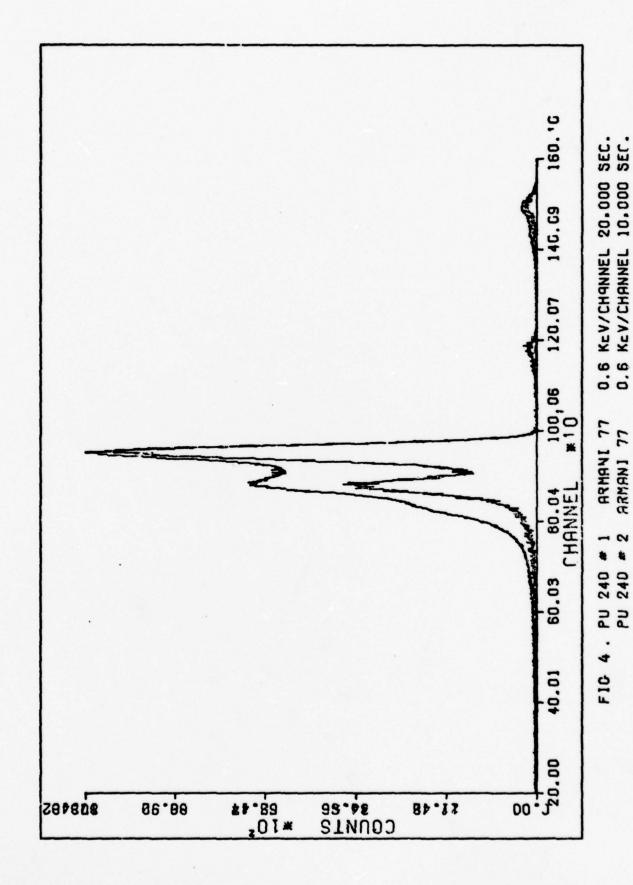
This study was specifically designed to be a continuation of work done by R. J. Hartley (Ref 5). He had prepared Program ALPHAFIT with the help of Dr. Philip Poirer from Program AUTOFIT which was written by J. R. Comfort of



0.6 KEV/CHANNEL 10 KSEC. FIG 2. AM 241 (ORTEC) UNBIASED RUN



11 (UNBXIDIZED) D.6 KEV/CHANNEL 40.000 SEC. # 13 (UNBXIDIZED) D.C KEV/CHANNEL 40.000 SEC. RA DEF . ო FIG



Argonne National Laboratory. AUTOFIT had been written to analyze gamma ray spectra and Hartley modified it to analyze alpha particle spectra. He then studied its behavior using computer generated Gaussian peaks and noted an anomaly in the computed error, which increased, dropped, and then increased again as the two peaks in the spectrum to be analyzed were set progressively closer together. He also used it to analyze samples of Am²⁴¹ and Pu²⁴⁰ using the spectrum from Po²¹⁰ as a reference curve shape. However, the results obtained showed large fluctuations in both the computed errors and the computed peak heights when either the sample of the same analyzed nuclide or the sample used as a reference was changed. These fluctuations were believed to be related to the variations in the source thicknesses.

Problem Statement

The problem is to develop a computer program that will take a spectrum from a multichannel analyzer, separate it into its separate components, and compute the quantities of the various nuclides present.

Plan of Attack

The basic approach selected was to modify Program

ALPHAFIT to use a library of curves with shapes representative of a range of source thicknesses. The program would then choose the curve with characteristics matching those of the source to be analyzed and use that curve as a

reference to analyze the spectrum of the unknown sample.

A set of reference samples were to be prepared using either Radium DEF or just Polonium²¹⁰ and reference spectra obtained from these samples. Also, the anomaly in the computed errors was to be studied and the program modified if necessary to correct the problem.

Summary of Work Done

The program was first modified to read data directly from magnetic tape or permanent disc storage. In order to reduce the core memory required and shorten the turnaround time, the program was changed from analyzing 20 peaks of 2048 channels each to analyzing 5 peaks of 512 channels. Subroutines to generate Gaussian peaks were then written and the program's behavior studied.

At the same time, a series of samples of Ra DEF was prepared with varying quantities of lead nitrate added to give samples of the same activity but varying thickness. An evaporative/precipitation technique developed by H. W. Kirby of the Mound Facility in Miamisburg, Ohio, was used to prepare these samples. An electroplating technique was also tried but sufficient time was not available to perfect it. The spectra from these samples were then recorded on magnetic tape and used to analyze spectra from existing samples of Am²⁴¹ and Pu²⁴⁰. However, the range of thicknesses was only appropriate for one of the plutonium samples. This sample was analyzed using the reduced version of the program and

analyzed again after the program was converted back to analyzing 2048 channels for up to 10 peaks. The results of these analyses confirmed the value of the library of curves approach.

Overview of Thesis

In this thesis, the theory pertinent to the analysis of alpha spectra is first discussed. Then, the equipment and procedures used are described. The results of the experiments are presented and analyzed. The changes to the program are explained. The results of the computer analyses are presented and discussed. Finally, the conclusions drawn from this study are set forth along with recommendations for future work.

II. Theory

The analysis of the amount of different nuclides by use of alpha spectrometry requires an understanding of the nature of the alpha spectra emitted by different nuclides, the processes which perturb the energy of the alpha particles emitted, and the response of the detector to the alpha particles. These are discussed in this chapter.

Alpha Decay

Alpha decay occurs as a transition from the nucleus of one of the heavy isotopes to a lower energy state in another isotope by the expulsion of a helium nucleus. Each parent nuclide emits alpha particles of certain specific energies, as listed in Table I. The exact energy released is determined chiefly by the quantum state of the resulting daughter nucleus. Once emitted, the alpha particle may lose varying amounts of energy by a number of processes up to and including detection.

If the emitting source material is extremely thin, some alpha particles may leave the source without losing any energy in collisions. However, if the source is even a few atoms thick, most alpha particles will lose some energy in ionizing collisions with the atomic electrons of the source material. The energy lost increases with the path length through the material which is the thickness of the material

Table I

Characteristics of Some Radioactive Isotopes
(Data from Lederer (Ref 10))

0.061 (max) 1.160 (max) 5.305 5.486 5.443 5.389	100 100 100 86 12.7 1.3
5.305 5.486 5.443	100 86 12.7
5.486 5.443	86 12.7
5.443	12.7
5.389	1.3
5.168	76
5.123	24
5.157	73.3
5.145	15.1
5.107	11.5
	5.157 5.145

divided by the sine of the angle between the path and the plane of the source surface. This energy loss is termed self-absorption.

A few alpha particles will initially be emitted away from the detector but will collide with a nucleus in the source itself or the source backing material. After a large change in direction and a large loss of energy in the collision, some of these particles will reach the detector and deposit their remaining energy. This is termed back-scatter.

Any material such as air between the source and the detector will absorb energy from the alpha particles, so alpha spectrometry should be conducted in an evacuated chamber.

When they reach the detector, the alpha particles may have to pass through a dead layer at the surface of the detector in which the electrons freed by collisions do not get collected to contribute to the pulse of current from the detector. As in self-absorption, the energy lost is dependent on the thickness of the dead layer and the angle of the particle's path through it.

Finally, the alpha particle reaches the active region of the detector, where it will lose its energy in collisions with electrons. These electrons produce a pulse of current which is amplified, shaped, and counted in a multi-channel analyzer.

Alpha Particle Interaction

The interaction of alpha particles with matter is strongly influenced by two characteristics of the alpha particle; its enormous mass relative to an electron mass $(M_{\pi} \approx 7000 \text{ m}_{\odot})$ and its double positive charge. The mass causes the alpha particle to travel in a virtually straight line except for Rutherford scattering with another nucleus. It also gives alpha particles a relatively low velocity for their high energy; for example, an alpha particle of energy 5 MeV has a speed only 3% that of light. An electron of the same energy would travel at 99% the speed of light. Thus an alpha particle has thirty (or more) times as long as an electron for its double charge to interact with an electron from each atom it passes. Alpha particles are easily stopped by only a thin layer of matter and may lose considerable energy before they even leave their source material.

The stopping power or specific energy loss dE/dX is given approximately by the following equation from Evans (Ref 40:637):

$$\frac{dE}{dX} = \frac{4\pi e^4 z^2}{m_0 V^2} \frac{N_A \rho}{GAW} z \left[\ln \frac{2m_0 V^2}{I} - \ln(1 - \beta^2) - \beta^2 \right]$$
 (1)

with

e = electronic charge

mo = electron rest mass

E = kinetic energy of the primary (alpha) particle

ze = charge of the primary particle

V = velocity of the primary particle

N_A = Avogadro's number

p = density of the material in grams per unit volume

GAW = the gram atomic weight of the element

Z = atomic number of the absorber

 $\beta = V/C$, where C = velocity of light in a vacuum

I = geometric-mean ionization and excitation potential for the absorbing atoms. This cannot be calculated accurately and is usually considered to be constant for each element. It must be determined experimentally for each element.

It is frequently more convenient to determine the loss per differential mass/area thickness traveled through. This is done by dividing both sides by ρ , the density. For a substance with several different elements such as lead nitrate, $Pb(NO_3)_2$, it is necessary to compute the energy loss for each element separately and then add the individual losses.

Alpha Particle Detection

This study deals with the detection of alpha particles by solid state surface barrier detectors. When an alpha particle enters the active region of the detector, the electrons with which it interacts and the holes left behind them move under the influence of the applied bias voltage. This gives a transient current which can be converted into a

voltage pulse and counted by the associated electronic
equipment. The height of this pulse can be expressed by the
following equation:

$$ph = [(E_{dep}/w) \times e \times \gamma]/C = N_e \gamma/C = q/C$$
 (2)

where

E_{dep} = energy deposited by the alpha particle

w = average energy required for the production of an electron-hole pair (eV/e-h pair)

e = electron charge (coulombs)

γ = charge collection efficiency. This is essentially .1 in detectors made of high quality single crystals.

 $N = E_{dep}/w = number of electron-hole pairs produced$

 $q = N_e \gamma = total charge collected (coulombs)$

C = capacitance of the detector (farads)

ph = pulse height in volts at the detector

These pulses are then amplified and shaped by the preamplifier, linear amplifier and biased amplifier and transmitted to a multichannel analyzer which counts the number of pulses with height between h and h $+\Delta h$ during the acquisition time. These are collected in a number of bins to form a pulse-height distribution.

Because of the statistical nature of the energy loss process, the pulses will be distributed over a range of channels or energies even if the alpha particles have

precisely the same energy when incident on the detector face. This statistical spreading is not caused by a distribution of either the original alpha energy or the energy deposited in the detector. It is caused by statistical variations in the number of electron-hole pairs created by each alpha particle as it deposits its energy in the detector. Additional spread in the pulse height distribution is caused by a spread in the energy of the alpha particles caused by self-absorption in the source material, the dead layer at the surface of the detector, and variations in the angle at which the alpha particle passes through the dead layer and the source. Further, though minor, contributions to the total arise from large angle scatters from the backplate of the source and the surroundings. These combine to give the tailing effect on the low energy side of the peak.

Electronic noise in the electronics also gives a slight increase in the spread but this will be the same for both the reference source and the unknown when they are analyzed with the same detector system.

Relation of Counts to Activity

Each unknown spectrum is analyzed to determine the number of peaks and the area of each peak. This area is the number of counts per channel summed over all of the channels. This is related to the source activity by the

following formula:

$$N_t/t_c = A \times G \times f_{ss} \times f_w \times E \times f_t \times f_\alpha$$
 (3)

where

N_t = total number of counts = the combined areas
 for all the peaks of each isotope

t = the counting time

A = the source activity

G = solid angle subtended by the active layer of the detector relative to the source

f_{ss} = surrounding scatter factor (negligible for α particles)

f_w = window factor, that is, absorption losses
 (generally = 1 for zero losses)

E = intrinsic efficiency of the detector in counts/
alpha (generally 1)

f_t = dead time correction (generally 1 for zero
 dead time)

 f_{α} = number of alphas per nuclear transformation

Need for Computer Peak Analysis

In alpha spectrometry, the energies and relative numbers of alpha particles emitted by each nuclide are assumed to be known from other studies, the results of which are compiled and tabulated in works such as Lederer (Ref 7). These works provide an outer bound on the set of possible nuclides, which can frequently be further restricted by other information about the unknown source. If only one

nuclide is present, then all of the nonbackground counts are from that nuclide and computer analysis is unnecessary. It is only in those cases where the relative numbers of nuclides are unknown, while the possible nuclides and energies and proportions of alphas emitted by each of those nuclides are known, that computer peak analysis is both necessary and feasible.

Computer Peak Analysis

Each spectrum is represented by an array $[A_i]$ which is the sum of a set of N components $Z_i(x_n)$, one for each of the N peaks. Each element in A is the sum of the corresponding elements of each component

$$A_{i} = \sum_{n=1}^{N} a_{n} Z_{i}(x_{n})$$
 (4)

where $Z_i(x_n)$ represents the counts in channel i from a source component that has its peak located at x_n . The locations, x_n , and relative strengths, a_n , are varied until a satisfactory fit of the test array [A] to the data array [Y].

Mathematically, this is accomplished by forming a chi-squared function

$$F = \sum_{i=1}^{N} (Y_i - A_i)^2 / (\omega Y_i)^2$$
 (5)

which is summed over the region being analyzed. The weighting function ωY_i is $\sqrt{10 + Y_i}$, where Y_i is the

ordinate of the im data point, that is, the counts in channel i. The inclusion of 10 slightly increases the weighting of the peak region relative to the tail and background and avoids division by zero.

Since Poisson statistics adequately describe the statistical fluctuations of the number of counts in each channel, the weighting function $(\omega_{i})^{2}$ is approximately equal to the variance. Thus, the chi-squared function represents the ratio of the observed spread in the analyzed data to the expected spread or variance.

The \mathbf{x}_n 's are determined by computing the function for locations to either side of \mathbf{x}_n and shifting the \mathbf{x}_n 's in the direction that reduces F. When a local minimum is found or when directed by the input data, that particular \mathbf{x}_n is fixed.

The a_n 's are then determined from direct solution of Eq (4) by matrix inversion techniques.

III. Experimental Equipment and Procedures

Introduction

This section covers the techniques and equipment used for alpha spectroscopy and the preparation and assay of the reference sources of Radium DEF.

Alpha Spectroscopy Equipment

The equipment used in these experiments consists of a vacuum chamber, surface barrier detector, power supplies and amplifiers, and multi-channel analyzers.

Vacuum Chamber. The vacuum chamber was a steel cylinder, 10 cm in diameter and 15 cm in height (See Figure 5). The cylinder is open at the top and is mounted around an 0-ring clamp to the top plate. There are four openings through the top plate. Two of these lead to gas valves. One valve is connected to the vacuum pump, while the other can be opened to the room air. The third is the mount and connection for the detector. A BNC connector above the plate is electrically connected through the plate to a threaded mount or microdot connector into which the detector is screwed. A BNC "L" connector leads directly from this to the preamplifier which is supported by a clamp and stand. The fourth opening is an O-ring fitting for a thin rod which is attached to a 3 cm x 3 cm horizontal plate

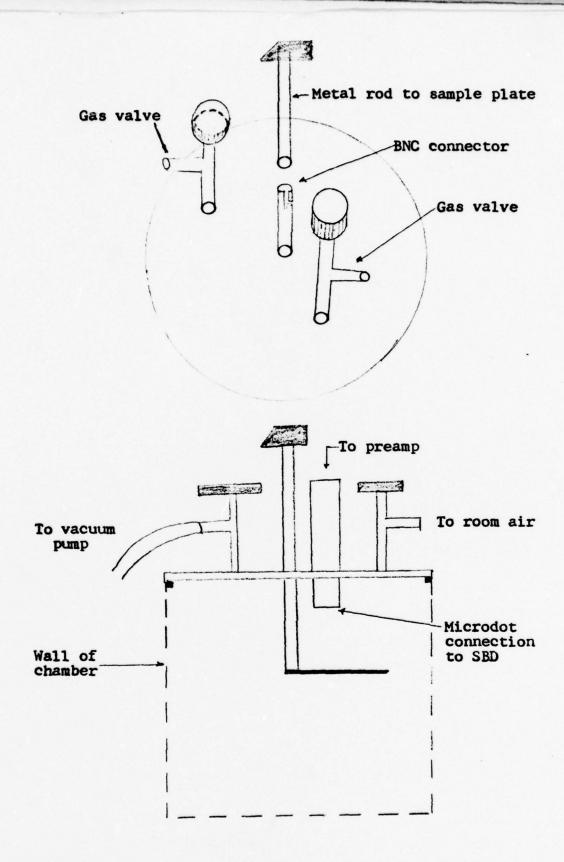


Fig. 5. Raised and Parallel Views of Vacuum Chamber for Alpha Spectroscopy (Not to Scale)

to hold samples. The distance from source to detector is varied by sliding this rod up or down.

<u>Detector</u>. An ORTEC 100 mm² surface barrier detector (SN 8-907A) with a microdot mount was used. This detector takes a maximum bias of 50.0 volts. A gross bias of 50 volts was applied for a net bias of 30-35 volts.

Amplifiers. The output from the surface barrier detector was fed, in turn, to an ORTEC Model 109-A preamplifier, a Tennelec Model TC203BLR linear amplifier, and an ORTEC Model 408 biased amplifier.

Multi-channel Analyzers. Two multi-channel analyzers were used to convert the output pulses into a count spectrum. An ND100 was used to obtain 512 channel spectra for preliminary observations. An ND2200 4096 channel analyzer was used to obtain 2048 channel spectra and record the results on magnetic tape. The tape was then taken to the central computer facility and stored there for use in computer analysis.

Assay Equipment

All of the radioactive samples prepared were assayed in an NMC 2m geometry gas flow proportional counter. The associated electronic equipment included a Hewlett-Packard 5554A preamplifier, an NIM Standard high voltage power

supply, a Tennelec TC203BLR linear amplifier, a Tennelec TC444 single channel analyzer, and a Canberra 1772 counter/timer.

Assay Procedure

The sample to be assayed was inserted into the flow counter, the counter sealed, and the air flushed out by the flowing gas. Each sample was then counted at least five times for one minute at each of two voltages, 1000V to count just alpha particles and 1600 or 1800V to count both alpha and beta particles.

Preparation of Sources

Kirby Method. Most of the sources prepared for this study were prepared by a method developed by H. W. Kirby of the Mound Facility in Miamisburg, Ohio (Ref 4:134-135). The backing plate is rinsed for a few minutes in alcoholic KOH, then rinsed with water and dried. The area for the sample is masked with a circular rod while the plate is sprayed with Krylon. The plate is then warmed and dried under a heat lamp for a few minutes. The uncoated area is covered with IN HNO₃ and allowed to stand for two minutes. The plate is then removed, rinsed thoroughly with distilled water, and dried again under the heat lamp.

The radioactive solution to be deposited is dropped on the uncoated area from a microsyringe and allowed to evaporate to dryness. This is then covered with two drops of 0.1 N HNO₃ and heated for two minutes without evaporating. One drop of 3N NH₄OH is then added and the solution is evaporated to dryness. Two or three more drops of NH₄OH are added and again evaporated to dryness. The NH₄OH is then driven off by further heating on a hot plate until the visible fumes are observed.

The major change from Kirby's procedure was to use a heat lamp for the initial drying operations. This was done because the available hot plates were not able to maintain a steady temperature in the 90-100°C region. However, eight of the first nine samples were prepared using hot plates.

Armani Electroplating Method. One sample was prepared using the "high voltage" electroplating procedure suggested by Roland Armani of Argonne National Laboratory (Ref 1).

One hundred microliters of the New England Nuclear Radium

DEF solution lot #72-187, about 0.1 microcurie, were added to 10 milliliters of 2-propanol in a 14 millimeter inner diameter glass tube, which was clamped with rubber washers at either end to a plate cleaned as for the Kirby method.

Platinum gauze was not available, so a roughly octagonal plate of platinum about six millimeters in diameter was used for the anode. The anode was immersed just below the surface of the plating solution, which was then plated for two hours at 600 volts and 1.1 microamps current.

Only about 30% of the Radium DEF was plated out and the resolution was no better than that of the evaporated samples. It was decided not to attempt to perfect this method and the remaining samples were all made by the Kirby method.

IV. Experimental Results

Introduction

This chapter covers the Ra DEF samples prepared as reference sources, the results of the assay to determine their activity, the spectra obtained from those sources, and the relative sharpness of the peaks obtained from those sources.

Sources Prepared

Twenty-one sources were prepared, assayed, and counted with the surface barrier detector. Sources 1 and 2 were prepared to test the Kirby method. Source 3 was prepared by electroplating. It gave the broadest peak of any of the sources and only 20% of the Ra DEF in the plating solution was plated onto the planchet, so the remaining sources were prepared by the Kirby method. Two sets of Ra DEF samples were then prepared with varying amounts of Pb(NO₃)₂ added to increase self-absorption.

Samples 4-9 were the first set of samples of varying thickness. The activities of these samples agreed within ±10%. However, as can be seen in Table II, the spread in the resulting spectra did not correspond to the quantity of added lead nitrate. Samples 7-9 were dried too long on the hot plate and this apparently caused considerable oxidation from the nitrate to the oxide. The spectra from samples 7-9

Table II

Comparison of Full Width at Half Maximum in 2048 Channel Biased Spectra From 100 mm²

Surface Barrier Detector with Quantity Added Pb(NO₃)₂ in the Sample

Sample	Added Pb(NO ₃) ₂ x .525µg + 3%	KeV FWHM Unoxidized	KeV FWHM Oxidized	α Act (Ox) α Act(Unox
1	0	39.1		
2	0	35.2		
3	0	51.6		
4	0	39.6		
5	1	52.0		
6	2	44.6		
7	3		24.3	
8	4		20.4	
9	5		28.1	
10	0	39.3	34.7	.90
11	0	30.2	29.2	.60
12	1	29.0	35.3	.89
13	2	37.1	34.3	.87
14	3	32.8	34.9	.92
15	4	35.4	35.9	.98
16	5	32.9	32.8	.87
17	5	35.6		
18	0	39.4		
19	0	31.9		
20	5	34.2		
21	5	37.1		

had the sharpest peaks of all, but they had double peaks due to ringing in the line from the amplifier to the multi-channel analyzer (This was corrected by inserting a terminator.) and were not used for computer analysis.

Samples 10-21 were the second set prepared with varying quantities of added lead nitrate. These were prepared simultaneously and dried under a heat lamp instead of on a hot plate. The lead nitrate was added in solutions of varying concentration so that the same volume of water was evaporated from each of the samples. Samples 1-17 were prepared on stainless steel planchets, while 18-21 were prepared on small squares of platinum. Sources 10-16 were later heated over a Fisher burner to oxidize the deposit from the nitrate to the oxide. These sources were used for the computer analyses.

Assay Results

All activities are calculated based on the NIC Radium DEF sample #AllO, with one microcurie equal to 2.22 x 10⁶ counts per minute. Sample AllO was measured at 514 disintegrations per second on 28 September 1961. The activity on 24 August 1978 is computed from the exponential decay law.

$$A(t) = A(t_0) \times e^{\frac{-(.693)(t-t_0)}{t_{1/2}}}$$

$$t_{1/2} = 20.4 \times 365 \text{ 1/4 days}$$

$$t_{-t_0} = 330 + 16 \times 365 \text{ 1/4 days}$$

$$A(t_0) = 514 \text{ dps } \pm 5\%$$

 $A(t) = 289 \text{ dps } \pm 5\%$

The remaining activities are calculated from the formula,

Activity (Sample) = $\frac{\text{Counts/min (Sample)} \times \text{Activity (Standard)}}{\text{Counts/min (Standard)}}$

As seen in Tables III and IV, which give the averages of five one-minute counts plus or minus the standard deviation of those counts, the unoxidized samples agreed fairly well in activity from sample to sample. As seen in Table IV, the standard deviations of the averages of activities for samples on the same backing (stainless steel or platinum) were only 1-2%. However, the combined $\alpha + \beta$ activity divided by three for the three nuclides in the decay chain was always several percent higher than the α only activity.

The results of the assay of samples 10-16 after oxidizing are listed in Table V. The combined $\alpha + \beta$ activity remained consistent from sample to sample. However, the fluctuation in α only counts increased to a standard deviation of 15% as varying amounts of polonium were driven off.

Spectral Results

The widths of the spectra from all the samples are compiled in Table II. There was no correlation between the amount of added lead nitrate in a sample and the full width at half maximum of the peak from that sample. Most of these

Table III Results of Assay of Samples 1-9 in 2π Geometry Gas Flow Proportional Counter at 1000V (α) and 1600V (α + β)

Sample	α Counts/60 sec	$\alpha + \beta$ cts/60 sec	Activity µCi	
			α	(a+s)/3
1	78,490 <u>+</u> 170	295,300 ± 2100	.0721	.0846
2	77,8 <u>0</u> 0 ± 230	336,920 <u>+</u> 640	.0715	.0966
3	21,730 ± 170	112,990 ± 290	.0200	.0324
4	122,640 ± 390	470,150 ± 780	.113	.135
5	122,570 ± 460	466,580 <u>+</u> 510	.113	.134
6	120,520 ± 3 <u>0</u> 0	474,200 ± 1300	.111	.136
7	102,030 ± 250	455,450 ± 470	.0938	.131
8	123,960 ± 220	483,180 ± 480	.114	.138
9	99,5 <u>0</u> 0 ± 3 <u>0</u> 0	402,830 ± 680	.0914	.115
A110	8,512 ± 92	27,291 ± 165	.00782 ±.00039	.00782

NOTE: Samples 1-9 were prepared on stainless stell planchets. Sample 3 was prepared by electroplating. Sample AllO was used as a calibration standard.

Table IV Results of Assay of Samples 10-21 in 2π Geometry Gas Flow Proportional Counter at 1000V (α) and 1800V (α + β)

Sample #	α Counts per 60 seconds	α + β Counts per 60 seconds	α Act μC _i	$(\alpha+\beta)/3$ Act μ C ₁
10	109,780 <u>+</u> 180	363,120 ± 560	.101	.104
11	107,470 <u>+</u> 230	359,490 <u>+</u> 8 <u>0</u> 0	.0988	.103
12	109,310 ± 2 <u>0</u> 0	373,910 <u>+</u> 660	.100	.107
13	111,740 <u>+</u> 170	377,640 ± 560	.103	.108
14	108,740 ± 310	371,480 <u>+</u> 520	.0999	.106
15	110,770 ± 320	369,880 <u>+</u> 670	.102	.106
16	108,450 <u>+</u> 280	352,250 <u>+</u> 850	.0997	.101
17	110,860 <u>+</u> 140	363,600 <u>+</u> 6300	.102	.104
18(p1)	116,210 ± 150	393,780 <u>+</u> 380	.107	.113
19(p2)	113,410 ± 450	390,340 <u>+</u> 490	.104	.112
20(p3)	115,090 ± 320	403,070 ± 470	.106	.116
21(p4)	113,730 ± 240	398,810 <u>+</u> 650	.105	.114
Average 10-17			.1008 ±.0014	.1049 ±.0023
Average 18-21			.1055 ±.0013	.1138 <u>+</u> .0017

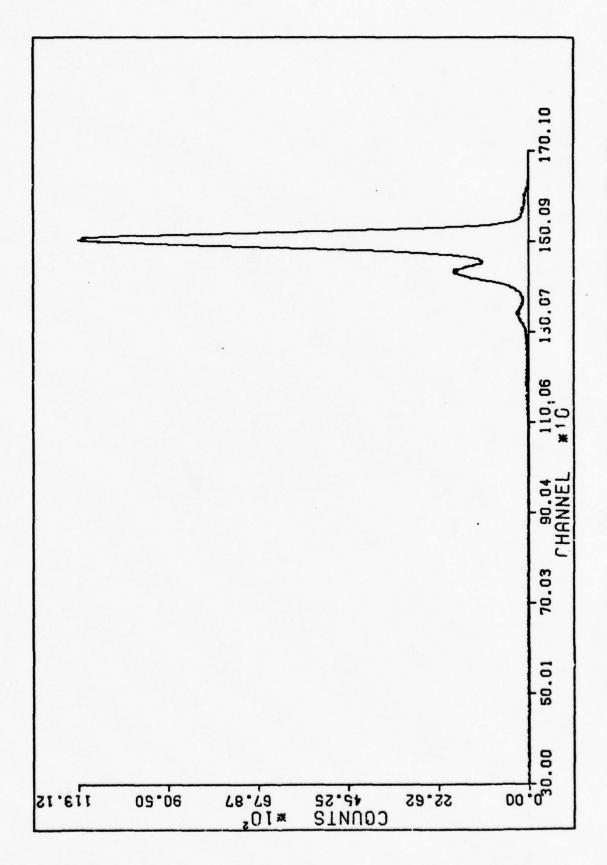
NOTE: Samples 10-17 were prepared on 1.25-inch diameter stainless steel planchets, while 18-21 were prepared on 14 mm square platinum planchets, which were then placed on stainless steel planchets for counting.

Table V Results of Assay of Samples 10-16 in 2π Geometry Gas Flow Proportional Counter at 1000V (α) and 1800V (α + β)

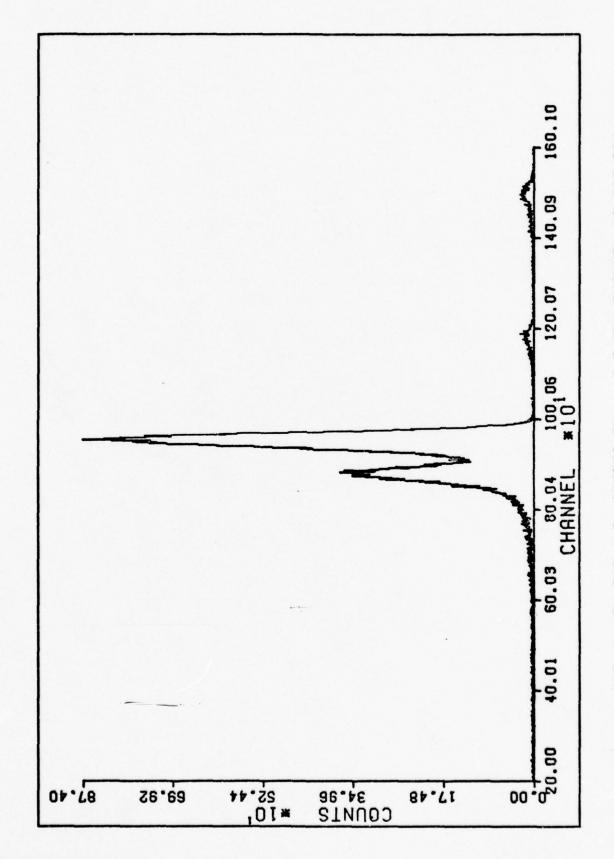
Sample #	α Counts per 60 seconds	α + β Counts per 60 seconds	Activity, $\alpha \mu C_{i}$	Activity, $(\alpha+\beta)/3$ μC_1
10	99,080 ± 460	381,680 <u>+</u> 120	.0911	.109
11	64,860 ± 220	342,390 ± 180	.0596	.0981
12	97,070 ± 240	367,080 ± 540	.0892	.105
13	97,3 <u>0</u> 0 ± 310	381,660 <u>+</u> 610	.0894	.109
14	99,860 ± 2 <u>0</u> 0	361,360 ± 510	.0918	.104
15	108,980 ± 310	371,930 <u>+</u> 790	.100	.107
16	94,260 ± 590	368,150 ± 480	.0866	.106
Average			.087 ±	.1054 ±

NOTE: These samples were gently heated over a Fisher burner to convert the deposit from the nitrate to the oxide.

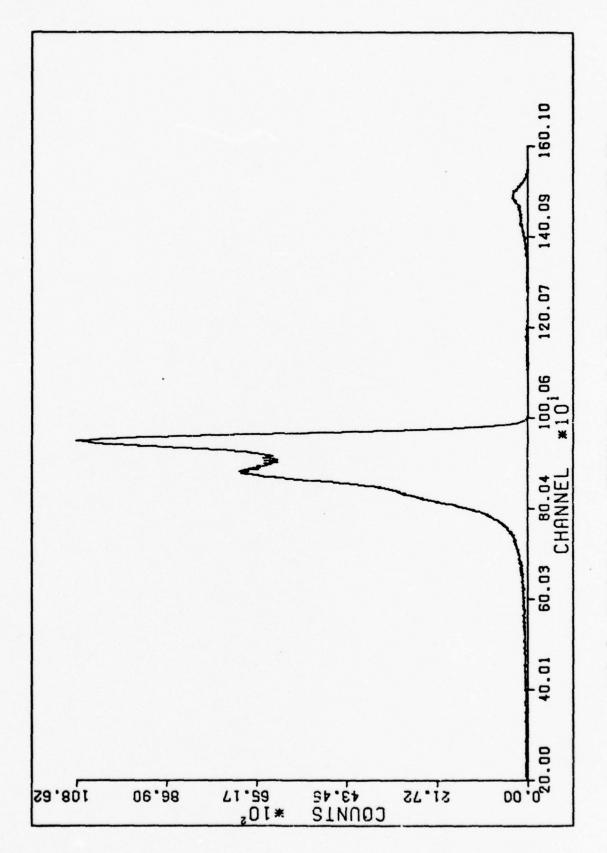
peaks were 10-15 KeV wider than the 21 KeV wide peaks from the Am²⁴¹ and Pu²⁴⁰ #2 samples, which are plotted in Figures 6 and 7. However, there was a good selection of widths in the region of Pu²⁴⁰ #1. Its full width at half maximum was about 32 KeV, but could not be determined precisely because the notch between the two main peaks did not come down to one-half the maximum (See Figure 7). Because of this good match, Pu²⁴⁰ #1 was selected as the "unknown" to be analyzed by the computer program using as reference peaks the spectra from the oxidized sources 10-16, which are plotted in Figures 8-15.



0.6 KEV/CHANNEL 10.000 SEC. **ORTEC 1/21/69** FIG 6 . RM 241



D.6 KEY/CHANNEL 10.000 SEC. FIG 7. PU 240 # 2 RRMRNI 77



0.6 KEV/CHANNEL 20.000 SEC. ARMANI 77 FIG 8. PU 240 # 1

Sell Market Sell

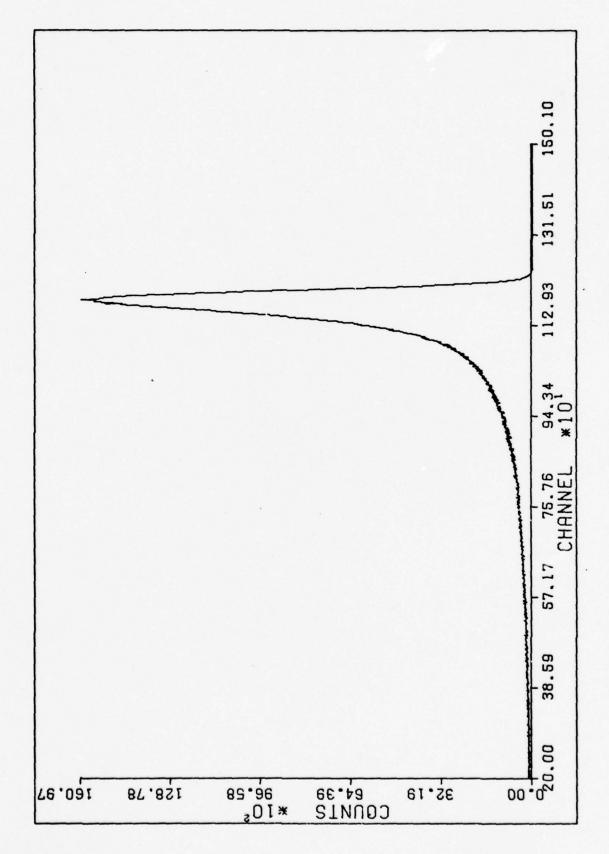


FIG 9. RR DEF # 10 (8XIB1ZEB) 0.6 KEV/CHRNNEL 40,000 SEC.

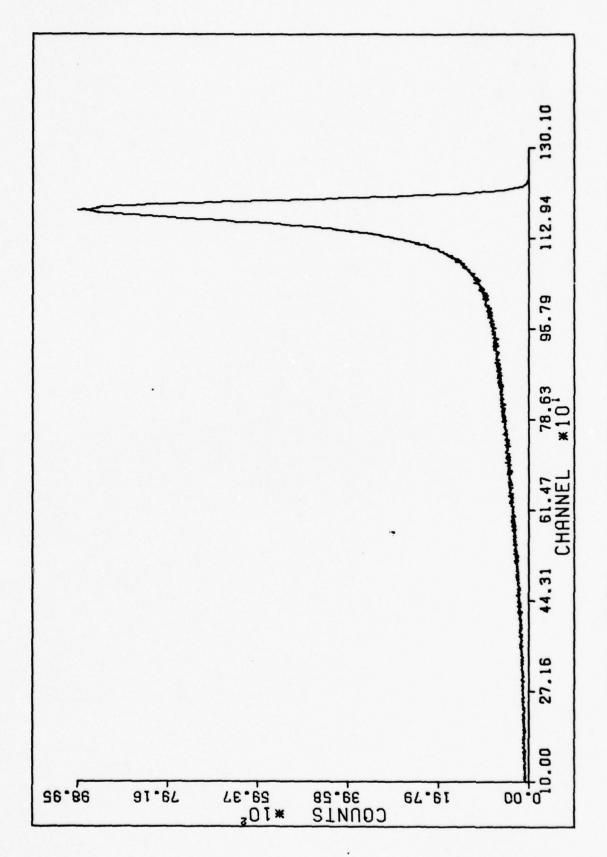


FIG 10, RA DEF # 11 (0XIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

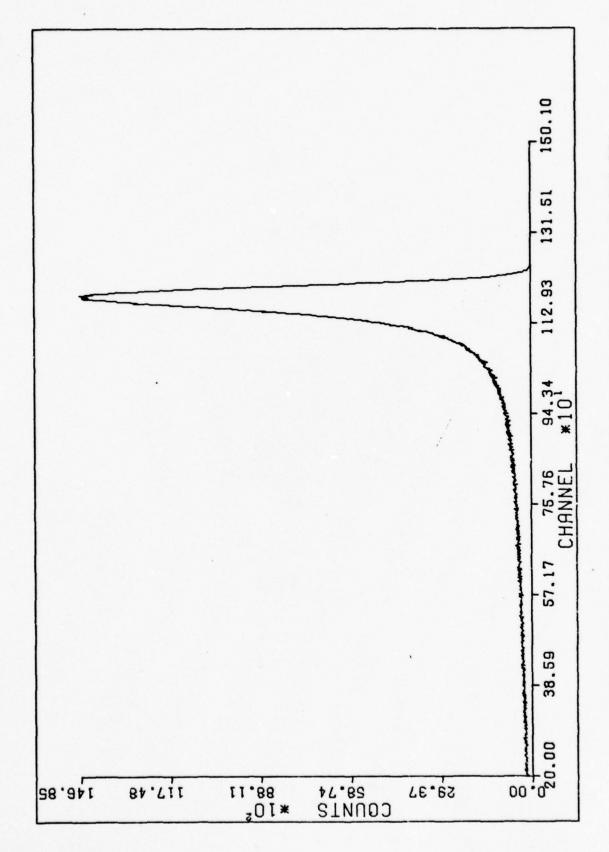


FIG 11. RR DEF # 12 (8X101ZED) 0.6 KEV/CHRNNEL 40,000 SEC.

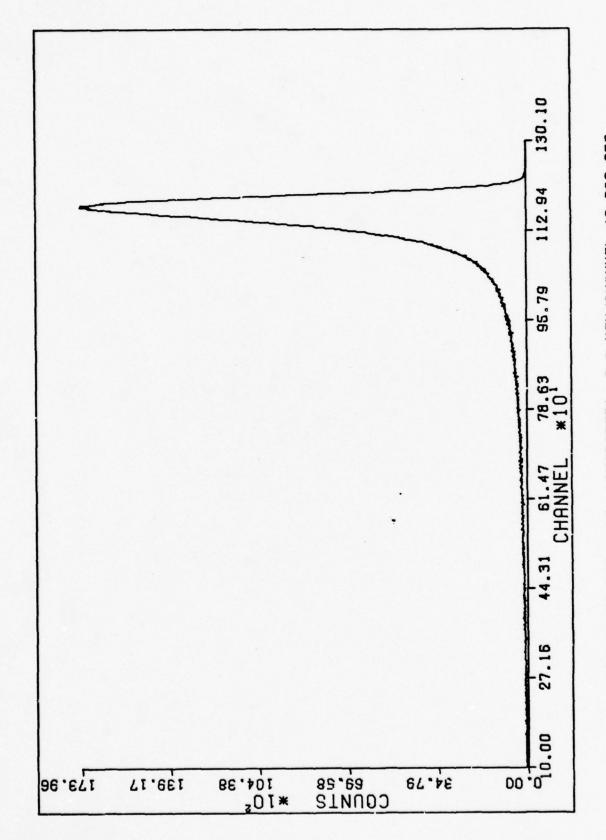


FIG 12, RA DEF # 13 (0XIDIZED) 0.6 KEV/CHANNEL 40,000 SEC.

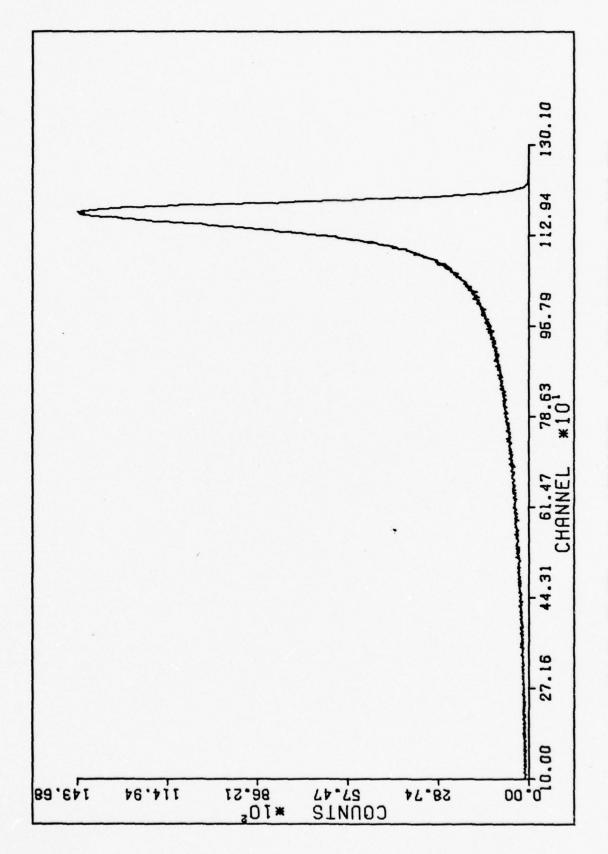


FIG 13, RR DEF # 14 (0XIDIZED) 0.6 KEV/CHRNNEL 40,000 SEC.

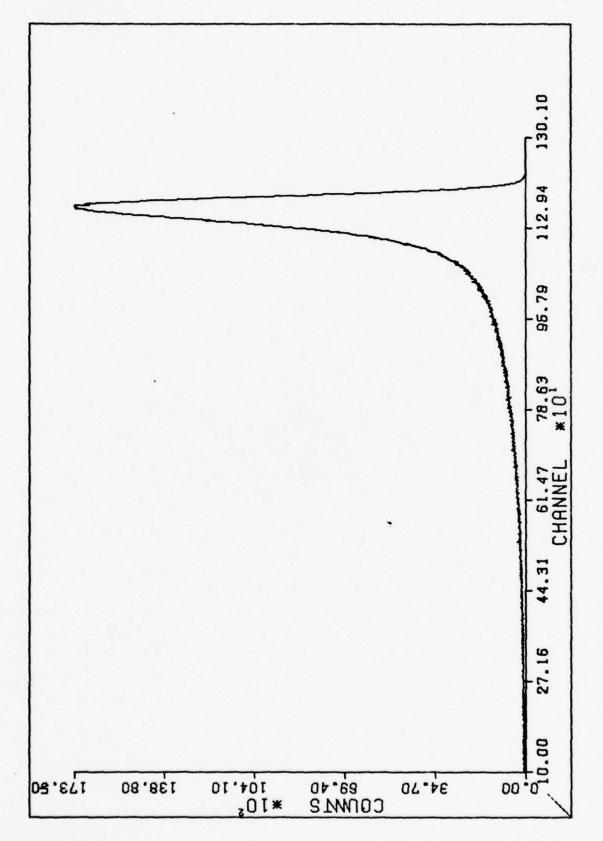


FIG 14. RA DEF # 15 (0X1DIZED) 0.6 KEV/CHANNEL 40.000 SEC.

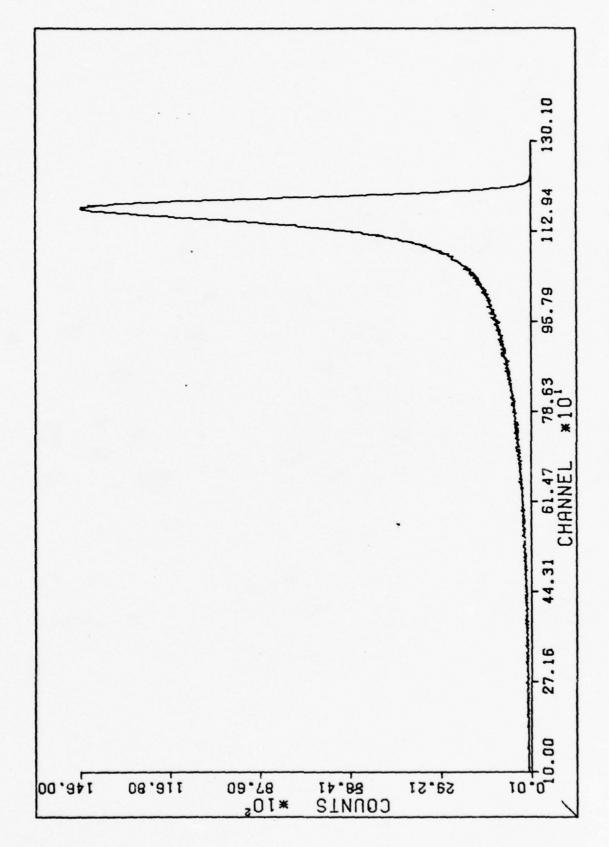


FIG 15. RR DEF # 16 (BXID1ZED) 0.6 KEV/CHRNNEL 40,000 SEC.

V. Program Modifications

Introduction

ALPHAFIT, which was produced by Lieutenant Richard S. Hartley with the help of Phil Poirier from Program AUTOFIT written by J. R. Comfort (Ref 5). Two specific modifications were originally planned, to convert the program to read the spectral data directly from magnetic tape or disc storage, and to use a library of curves to choose the curve which will give the best analysis and use it to analyze the unknown spectrum. In addition, subroutines were written to create Gaussian spectra modified by a Poisson distribution for counts in each channel and these spectra were used in place of detector spectra to study the program's performance.

Conversion to Tape

It was desired to convert the program to read the spectral data directly from the magnetic tape on which they were written by the multi-channel analyzer. Two programs, SCRIPT and SPECTRA were written by H. Careway (Ref 3) to use the FORTRAN BUFFER IN and DECODE statements to read these data into an array. SCRIPT then prints out the numbers, while SPECTRA produces a CALCOMP plot. The READ section of these programs was extracted and modified into subroutine RDSPEC. RDSPEC was then called directly from the main

program to read the reference spectra and from subroutine SPCTRM to read the unknown spectrum.

Reading the data in this manner is not without difficulty. First, the spectra to be read must be placed in order on file TAPE1 by using the SKIPF and COPYCF control card statements. Then, the statement FILE, TAPE1, FO=SQ, BT=C, RT=S, BFS=1000. is used to tell the computer this is a stranger tape (RT=S) and the buffer size (BFS=1000). This must be followed by a LOAD-SET statement such as LDSET, FILES=TAPE1. PRESET=ZERO.

Second, perhaps because of a stray bit or an unclean tape, a datum would be rejected by the computer dumping the program immediately. RDSPEC was modified with the statement, ERRSET (KOUNTS, 100), so that the program would not dump for just one such datum. The numbers read in this way were always satisfactory, but occasionally the bottom section of a spectrum would be rejected by the computer.

Reorganization

Program ALPHAFIT analyzed spectra of 2048 channels for up to 20 separate peaks. This is necessary for analyzing a spectrum with several isotopes over a wide range of energies but requires an enormous (over 250K) quantity of core storage. This requirement impedes studying the behavior of the program, making changes, and troubleshooting, so the program was reduced to analyzing 512 channels out of the 2048 containing up to five peaks. This reduced the

each evening. However, this reorganization imposed certain limits. With the biased amplifier spreading the spectrum out to 0.48 or 0.60 KeV per channel, a range of only 250-300 KeV could be studied. This was adequate for Am 241 but insufficient for the Pu 240 spectra taken, so only the two largest peaks in Pu 240 were analyzed. More than five peaks would have to be analyzed in most unknown spectra.

The second change was to have the program read and store five reference spectra to analyze each unknown spectrum. This was done simply by copying each spectrum into the array REFSTO (520.5) before using the reference to analyze the unknown.

Artificial Spectra

In order to study the performance of the program's analyzing routines, it was desired to generate spectra of arbitrary characteristics to simulate alpha spectra. Subroutine CONJUR was written to use several routines written by Bevington (Ref 2) to generate Gaussian peaks of specified height, standard deviation and position, add them to create a spectrum, then randomly modify the counts in each channel according to an approximate Poisson distribution. CONJUR and the associated subroutines were then substituted for subroutine RDSPEC. The resulting program was called ALFAIC.

VI. Program Computation Results

Introduction

The program's analyzing performance was extensively tested under idealized conditions by using generated Gaussian type spectra. Samples of americium and plutonium were analyzed by the 512 channel version using the best of the samples prepared (after oxidizing). One of the plutonium samples was also analyzed using the 2048 channel version of the program. These analyses showed that a difference of only one channel between the widths of the reference and unknown peaks caused significant reduction in the accuracy of the analysis.

Conjured Spectra

The program was used to analyze spectra composed of two Gaussian peaks with a standard deviation (σ) of 20 channels. The separation between these peaks was varied from one quarter to two and a half times the standard deviation (5-50 channels) to investigate the anomaly reported by Hartley (Ref 5:22). The width of the reference peak was varied from 15 to 25 channels to observe this effect.

Separation Effect. The program was tested with peaks of 5:10 and 1:10 relative heights (Tables VI and VII). None

Table VI

Errors Versus Separation Distance for Gaussian
Peaks 1/2 = 5:10, σ = 20, Peak 1 in
Channel 250, True Area ≈ 572000

Area(true) %	RMS Error %	E	imated rror , Peak 2	Ratio Peak 2 Peak 1
.064	.035	805	865	.238
.065	.038	525	543	1.933
.065	.037	355	390	2.358
.062	.051	313	357	2.233
.0604	.046	254	301	2.120
.0581	.035	196	236	1.986
.0538	.033	164	209	2.007
.0480	.035	152.5	202.4	2.0008
	.064 .065 .065 .062 .0604 .0581	.064 .035 .065 .038 .065 .037 .062 .051 .0604 .046 .0581 .035 .0538 .033	.064 .035 805 .065 .038 525 .065 .037 355 .062 .051 313 .0604 .046 254 .0581 .035 196 .0538 .033 164	.064 .035 805 865 .065 .038 525 543 .065 .037 355 390 .062 .051 313 357 .0604 .046 254 301 .0581 .035 196 236 .0538 .033 164 209

Table VII

Errors Versus Separation Distance for Gaussian
Peaks 1/2 = 1:10, σ = 20, Peak 1 in
Channel 250, True Area ≈ 417000

Center Peak 2	Area(true)-Area(comp) Area(true) %	RMS Error %		timated Error 1, Peak 2	Ratio Peak 2 Peak 1
255	. 084	.043	285	222	.0047
260	.079	.079	348	218	.012
265	.087	.129	173	460	81
270	.078	.045	169	236	10.7
275	.075	.044	134	211	10.3
280	.072	.043	107	191	10.2
300	.083	.043	78	195	10.04
350	.049	.042	52	161	10.06

of these peaks were sufficiently separated to show a drop in counts between the two peaks (Figures 16-17). (Compare with the americium and plutonium spectra in Figures 6 and 8.)

The absolute difference between the computed and true areas rises gradually as the two peaks approach. When the peaks are separated by less than one standard deviation, the Root Mean Square difference between the computed approximation and the analyzed spectrum declines as the smaller peak vanishes into the larger, while the computed error in each peak is generally larger and the computed ratio of the two peaks fluctuates wildly.

These results show the program is unable to resolve two peaks accurately when they are so close as to appear to be one (See Figure 18). Nevertheless, both the difference between the absolute areas of the unknown and resolved spectra, the absolute residual, and the Root Mean Square of the difference at each point, the average residual, remain less than 0.1%. The two peaks have merged and are indistinguishable. The only indication that the spectrum is composed of more than one peak is the 1-10% difference between the left and right half widths at half maximum.

Reference Width Effect. The analysis of peaks of fixed width with references of various widths show (See Tables VIII and IX and Figures 19-20) that matching the spread of the reference to that of the unknown can reduce the residuals

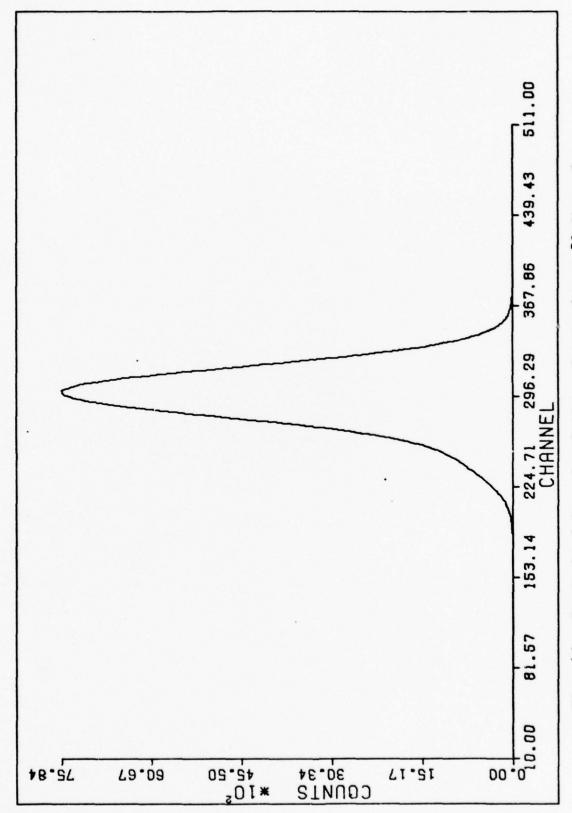
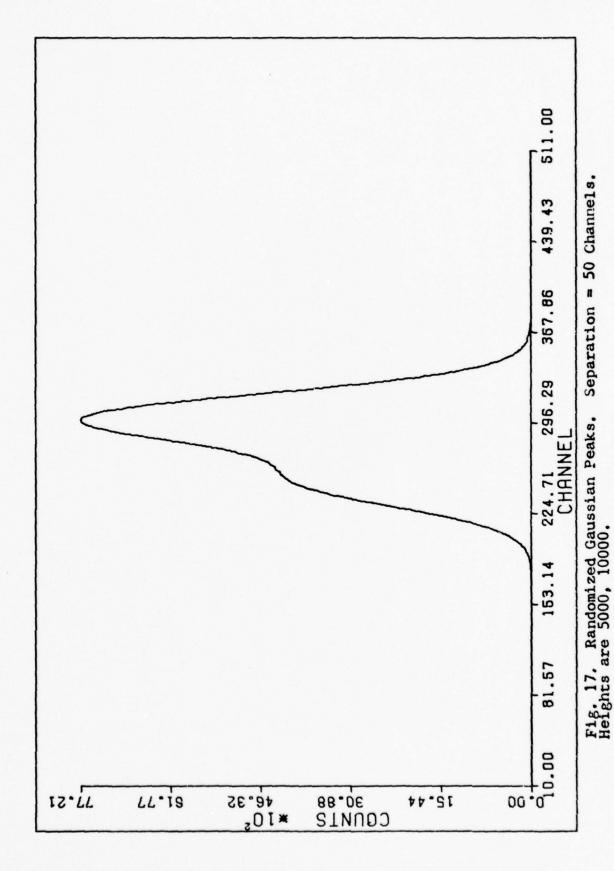


Fig. 16. Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 1000, 10000.



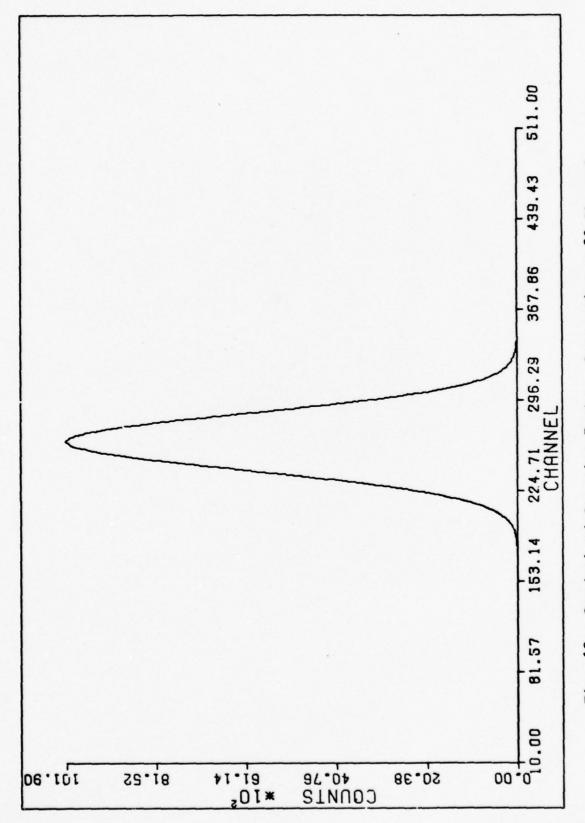


Fig. 18. Randomized Gaussian Peaks. Separation = 20 Channels. Heights are 5000, 10000.

Table VIII

Analysis of (σ = 20) Gaussian Peaks with Reference
Peaks of Varying σ. Ratio of Peak
Heights = 10:1 Separation = 50(2.5 σ)

True Area		
-Resolved Area	RMS Error	Resolved Ratio
2092	10299	7.1
1175	7857	7.6
134	3570	8.6
296	1374	7.9
4.2	703	8.8
237	171	10.05
353	761	11.1
436	1492	12.3
564	2954	13.5
731	5363	18.3
703	11297	-66
	2092 1175 134 296 4.2 237 353 436 564 731	2092 10299 1175 7857 134 3570 296 1374 4.2 703 237 171 353 761 436 1492 564 2954 731 5363

Table IX

Analysis of (σ = 20) Gaussian Peaks with Reference
Peaks of Varying σ . Ratio of Peak
Heights = 10:5 Separation = 50(2.5 σ)

Reference σ	True Area -Resolved Area	RMS Error	Resolved Ratio of Two Peaks
15	4392	13127	1.72
16	2527	10130	1.77
18	623	4724	1.88
19	6.4	1926	1.939
19.5	168.6	964.8	1.9699
20.0	272.8	198.4	2,0008
20.5	394.6	927.8	2.046
21.0	500.2	1728.3	2.11
22	678	4154	2,23
24	952	7856	2.56
25	1072	9580	2.76

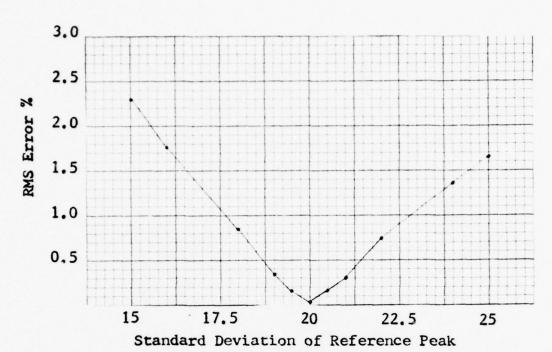


Fig. 19. Analysis of $(\sigma = 20)$ Gaussian Peaks with Reference Peaks of Different Widths. Ratio of Peak Heights = 10:1.

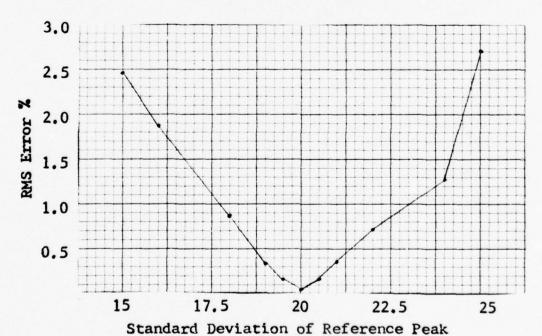


Fig. 20. Analysis with Reference Peaks of Different Widths. Standard Deviation of Peaks Analyzed = 20. Ratio of Peak Heights = 10:5.

by two or three orders of magnitude under ideal conditions.

A difference of only 0.5 in the standard deviation produces
a clear increase in the RMS error.

Real Spectra

512 Channel Analyses. The first group of analyses were conducted on a 512 channel segment out of the full 2048 channel spectrum. Five spectra were used to analyze two samples, Am²⁴¹ and Pu²⁴⁰ #1. The spectra from the oxidized Ra DEF samples 10, 11, 12, 13, and 16 were selected because they had the sharpest peaks. Although these peaks could not be placed in sequence showing a continuous regular change in the curve shape, they could be placed in order of their full width at half maximum. As shown in Table X and Figures 21 and 22, the RMS error corresponded directly to the fit between the FWHM's of the unknown and the reference used for analysis. It first dropped and then rose as the FWHM increased for the plutonium sample and rose steadily for the americium sample.

Other measurements of the accuracy of the fit were not as well correlated to the FWHM. The difference in areas when analyzing Pu^{240} #1 showed the same trend as the RMS error except for sample #10, but there was no agreement when analyzing americium. The computed ratio of the two main peaks in Pu^{240} was too low except for sample 16.

2048 Channel Analyses. The analyses on the full 2048 channel spectrum of Pu²⁴⁰ showed good correlation between

Analysis of Plutonium and Americium with Polonium Spectra of Varying Self-Absorption. All Spectra from 100 mm² ORTEC Surface Barrier Detector at 30-35 V Net Bias

Unknown = Pu ²⁴⁰ #	1		FWHM = a	bout 32
Reference Spectrum from Sample #	FWHM (KeV)	∆ Area Error (counts)	RMS Error (counts)	Computed Ratio
11	29.2	9318	11244	2.79
16	32.8	7833	10618	3.06
13	34.3	7206	6943	2.42
10	34.7	23038	5942	2.67
12	35.3	7773	9616	2.71
Unknown = Am ²⁴¹			FWHM = 2	1.1
Reference Spectrum from Sample #	FWHM (KeV)	∆ Area Error (counts)	RMS Error (counts)	
11	29.2	29140	18325	
16	32.8	24330	20954	
13	34.3	15630	21835	
10	34.7	9642	21709	
12	35.3	19826	23368	

NOTE: Only 512 channels of these spectra containing the two or three chief peaks were analyzed. The ratio for plutonium is for the 5.168 and 5.123 meV peaks. The true ratio is 3.167.

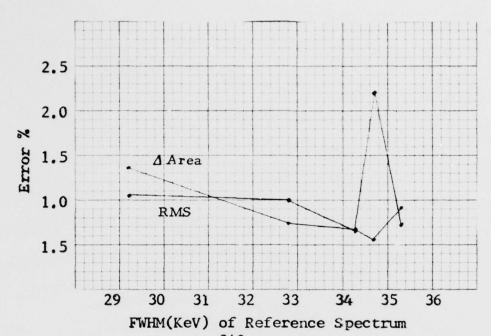


Fig. 21. Analysis of Pu 240 #1 with Various Ra DEF Samples. All Spectra From ORTEC 100 mm 2 SBD at 30-35 V Net Bias.

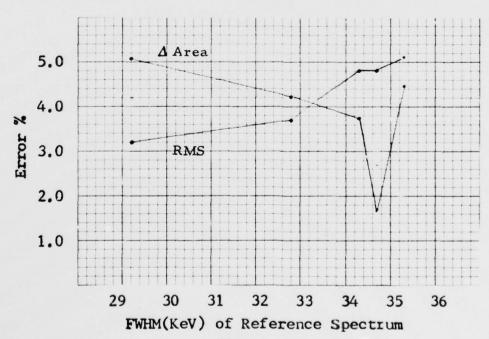


Fig. 22. Analysis of Am²⁴¹ with Various Ra DEF Samples. All Spectra From ORTEC 100 mm² SBD at 30-35 V Net Bias.

all three measures of the fit and the match of the FWHM's except for reference sample #15 (See Table XI and Figure 23). This had the largest FWHM but gave the second best fit. The resolved composite areas were 50% to 150% too large and the composite now gave too large a percentage of the counts to the largest peak. These results confirm that matching the reference curve shape to the spectrum being analyzed gives a more accurate analysis.

The results of these analyses show the potential of the library of curves approach to produce a more accurate analysis of alpha spectra. However, the program remains unstable and capable of producing bizarre results even under good conditions. The peak locating routines will sometimes shift the locations of two clearly separated peaks to only a few channels apart and at other times will shift one or more peaks completely out of the spectrum. The routines which compute the relative multipliers for each peak (See Eq (4)) will at times return a negative value for one of the peaks. These problems need to be solved in future work with this program before it can be considered completely reliable. Even then, the program's performance will be limited by the reference spectra available.

Table XI Results of 2048 Channel Analyses of Pu 240 #1

Pu^{240} FWHM = 103.58 Channels				
Reference Sample	FWHM Channels/KeV	Δ Area Counts/%	RMS Counts/%	Peak Ratio
110x	50.68/29.2	1624448/142	75965/6.6	16.4
160x	57.07/32.8	1033675/90	53577/4.7	7.3
130x	59.59/34.3	551953/48	37264/3,25	4.42
100x	58.05/34.7	902232/79	46422/4.05	5.8
120x	60,59/35,3	1203889/105	63790/5.6	17.4
140x	60.63/35.3	1375767/120	63419/5.5	12.4
150x	62.47/36.4	831737/73	43413/3.8	4.98

NOTE: The peak ratio is for the 5.168 and 5.123 meV peaks. The true ratio is 3.167.

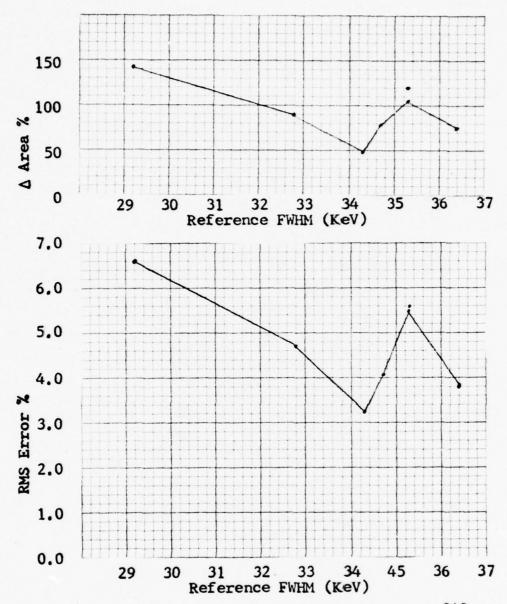


Fig. 23. Results of 2048 Channel Analyses of Pu^{240} #1 with Various Ra DEF Samples. All Spectra From ORTEC 100 mm² SBD at 30-35 V Net Bias.

VII. Conclusions and Recommendations

Conclusions

The analyses with generated spectra clearly show that, at least under ideal conditions, matching the FWHM of the reference peak to the FWHM of the spectrum to be analyzed gives a better analysis. Differences of only one channel in these FWHM's were shown to increase the RMS error by a factor of 3 to 5. This strongly supports the need for a library of reference curves to use in analyzing various alpha spectra.

The analyses with real spectra also support these conclusions. The reduced range (512 channel) analyses of americium and plutonium both show a reduction in the RMS error as the FWHM of the reference peak is made closer to the FWHM of the spectrum analyzed. The full range (2048 channel) analyses of plutonium confirm this reduction of the RMS error and, in addition, show a corresponding reduction in the absolute residual area and more accurate resolution of the relative areas in the two chief peaks.

These analyses show that the use of a library of reference spectra can give a several percent reduction in error provided that reference spectra with the correct characteristics are available. The chief need at this time is for a consistent set of smoothly varying spectra,

including a range of FWHM's as low as 20 KeV or better.

Recommendations

Samples. The main need is for better reference samples. Po²¹⁰ is clearly the isotope to use. It may be possible to prepare adequate Ra DEF samples, but these will have to be the oxide or perhaps bare metal. The nitrate samples have too much self-abscrption, even with no added lead. An electroplating technique will probably be required to produce samples with low enough self-absorption.

There are two further studies that could be made with the samples prepared for this thesis. New spectra should be obtained from samples 7-9. If the peaks from these have FWHM's as narrow as indicated in Table II, they should be used to analyze samples with correspondingly low selfabsorption such as the americium²⁴¹ sample used in this study. Additional spectra from the later set (10-21) should also be taken in another year or two to check for changes in the curve shapes due to a more even distribution in the polonium²¹⁰ as a result of radioactive decay.

<u>Program.</u> There are also improvements that can be made in the program. A big problem is how to store and access a large library of 2048 channel reference spectra. These will probably have to be stored on magnetic tape, so some means of conveniently reading a particular record is needed.

The operation of the main program could be considerably streamlined by eliminating some of the unused options. The following sequence should be adequate. First, controlling data are read. Second, the spectrum to be analyzed and a background spectrum are read. The FWHM is computed for the largest peak in the unknown spectrum and a reference spectrum is selected and read. The program then passes these three arrays to the analysis routines and conducts the analysis. The automatic and interpolated background options and the computer-derived peak shape options could then be eliminated.

It would also be useful to modify the analyzing routines so that the spectrum for each peak extends all the way to zero, perhaps using a computed average of the lower channels to fill the gap from the bottom channel down to zero. Finally, the analysis routines should be carefully studied to verify their correct operation and make useful modifications such as rejecting negative peaks and limiting the shifting of the specified peaks to a fixed range about the specified location. These routines are the subroutines PREPAR and DAVIDN and all the subroutines called by these two.

Bibliography

- Armani, Roland. Private communication with Dr. George John. 18 August 1978.
- 2. Bevington, Philip R. Data Reduction and Error Analysis for the Physical Sciences. New York: McGraw-Hill Book Company, 1969.
- 3. Careway, Harold A. Energy Dispersive X-ray Analysis of Heavy Elements. AFIT-GNE-75-2. Wright-Patterson AFB, Ohio: Air Force Institute of Technology, March 1975.
- 4. Evans, Robley D. The Atomic Nucleus. New York: McGraw-Hill Book Company, 1955.
- 5. Hartley, Richard S. A Computer Code to Analyze Alpha Spectra. AFIT-GNE-78M-5. Wright-Patterson AFB, Ohio: Air Force Institute of Technology, March 1978.
- 6. Kirby, H. W. and J. J. Dauby. "Preparation of Sources for Alpha Spectrometry," Sanderdruck aus Radiochimica Acta, 5: 133-137 (1966).
- 7. Lederer, C. Michael, Jack M. Hollander, and Isadore Perlman. <u>Table of Isotopes</u> (Sixth Edition). New York: John Wiley and Sons, Inc. (March 1968).

Appendix A

Utility Programs

Introduction

Several programs besides ALPHFT (alpha fit) were used during the work on this thesis. It was decided to read the multi-channel analyzer generated data from magnetic tape (or tape-derived permanent disc) storage. Captain Harold A. Careway (Ref 3) had written two programs, SCRIPT and SPECTRA, to perform this operation using the FORTRAN BUFFER IN and DECODE statements.

Program SCRIPT

Program SCRIPT was designed to read in a series of L consecutive spectra, then print out the first IC channels of each spectrum. In the form developed by Careway, both SCRIPT and SPECTRA were quite sensitive to some phenomenon which caused the code for a number to be interpreted as the code for {, @, ", or some other character. This would cause the computer to dump the program without reading, writing, or plotting any more spectra. At the suggestion of Captain Stinson, these programs were modified using the CALL ERRSET statement to allow the computer to accept a few such events before dumping the program. This allowed subsequent spectra to be read and written or plotted on the

same computer run. By printing out only the first few lines from a spectrum, program SCRIPT could easily be used to investigate which spectra contain bad data. However, when the full spectrum was printed out after such an occurrence, no bad data were observed.

Program SPECTRE

Program SPECTRA, the plotting routine, was extensively modified so that it could be used to plot the graphs for this thesis. It was then renamed SPECTRE. In the original form, it generated only a large graph of variable dimensions similar to the type 2 plot in SPECTRE but with no title. The program always plotted channels 70 to IC, an input variable. The spectra to be plotted had to be placed in order on the file TAPE1 by correct use of the SKIPF, COPYCF, and REWIND control cards. Provision was made to edit erroneous data prior to plotting.

Modifications

The program was first modified using CALL ERRSET as was SCRIPT. It was then modified using additional CALL PLOT statements and a CALL SYMBOL statement to generate a smaller plot enclosed in a box with boundaries marked for cutting with a title at the bottom of the page (after cutting). The titles were initialized in the array ITITLE by a series of DATA statements and the correct title was determined from the tagword of the data to be plotted. Finally, the program was heavily modified to allow the user to read the 4XN array

NTAG, which specified the spectrum/tagword to be plotted, a choice of the old and new formats, and the first and last channels to be plotted. It is still desirable to register the first spectrum to be plotted by using the SKIPF control card in order to reduce Input/Output time, but this is not necessary. The tagwords to be plotted may be read in any order but will be plotted in ascending order.

Appendix B

Program SCRIPT

```
PROGEAM SCRIPT (INPUT, CUIPUT, TAPE1)
      DIMENSION Y (4100), X (256), MW (160)
C THIS PROGRAM PRINTS OUT SPECTRA
C THE FIRST SPECTRA TO BE PRINTED OUT MUST BE REGISTERED BY USE OF
C THE SKIPF CONTROL CARD
C THE FIRST DATA CARD IS IS FORMAT *****
                                            L= NUMBER OF SPECTRA
C THE SECOND DATA CARD IS IS FORMAT **** IC= NUMBER OF CHANNELS
   READ 1000, L
      READ 1000, IC
      DO 100 J=1, L
      N=1
      KK=1
      BUFFER IN (1,0) (MM(1), MM(160))
 10
      KK=UNIT(1)
      CALL ERRSET (KOUNT, 190)
      DECODE (100,50, HW) 4, 44, X
      IF (KOUNT.GT.0) GO TO 100
      FORMAT(2X,11,2X,44,23Ff.0,9(/25F5.0),/,8F5.0)
 50
      DO 80 J=1,256
      Y(N) = X(I)
 80
      N=N+1
      IF (KK . NE . 0) GO TO 10
      PRINT*," UNIT(1) = ", KK," N = ", N
      PRINT 1010, 4
      NN = (IC/10) + 1
      DO 90 K=1,NN
      IN= (K-1) 10
      TT=I+ +1
      PRINT 1020, IN, Y(II), Y(II+1), Y(II+2), Y(II+3), Y(II+4), Y(II+5), Y(II+
     C6) .Y(II+7) .Y(II+8) ,Y(II+9)
 30
      CONTINUE
      CONTINUE
 100
 1000 FORMAT (13)
 1010 FORMAT (141, T51, "TAGHORD NUMBER", [55, [5]
 1020 FORMAT (1X, I5, 10F10.0)
      STOP
      END
```

Appendix C

User Instructions for SCRIPT

Program SCRIPT is simple to use. The spectra to be read are placed on file TAPE1. The FILE and LDSET statements tell the computer the buffer size for the file and load it to be read. Two data cards are required in I5 format. The first should contain L, the number of spectra to be read and printed. The second should give IC, the number of channels to be printed out for each spectrum starting with channel 0. A typical control card sequence would be the following. FTN.

ATTACH, TAPE1, XFILE, MR=1.

FILE, TAPE1, FO=SQ, BT=C, RT=S, BFS=1000.

LDSET, FILES=TAPE1, PRESET=ZERO.

LGO.

Appendix D

Program SPECTRE

```
PROGRAM SPECTRE IS AN ELABORATED VERSION OF PROGRAM SPECTRA,
        WHICH WAS PROVIDED BY DR. GEORGE JOHN.
        IT ALLOWS THE PLOTTING OF TWO DIFFERENT PLOTS INTERCHANGEABLY:
C
             ONE IS A SMALL BORDERED PLOT IN AFIT THESIS FORMAT.
C
             THE OTHER IS A LARGER VERSION, WHICH MAY BE MORE SUITABLE
C
             FOR DIRECT COMPARISONS.
C
     DIMENSION X(4100), Y(4100), 7(256), 44(160)
     DINENSION ITITLE (6.100)
     DIMENSION NTAG(4,20), XA(2), YA(2)
DATA ITITLE(1,42)/60HFIG
                                . RA JEF # 17 (JNOXIDIZED) 0.6 KEV/CHAN
     CNEL 10030 SEC. /
     DATA ITITLE(1,43)/60HFIG
                               . RA DEF # 17 (JNOXIDIZED) 0.6 KEV/CHAN
    CNEL 40000 SEC. /
     DATA ITITLE(1, 44)/60HFJG
                               . RA DEF # 13 (JNOXIDIZED) 0.6 KEV/CHAN
     CNEL 10000 SEC. /
     DATA ITITLE(1,45)/60HFIG
                                . RA JEF # 13 (JNOXIDIZED) 0.6 KEV/CHAN
     CNEL 18000 SEC. /
                                . RA JEF # 13 (JNOXIDIZED) 0.6 KEV/CHAN
     DATA ITITLE(1,46)/60HFIG
     CNEL 10000 SEC. /
                                . RA JEF # 19 (JNOXIDIZED) 0.6 KEV/CHAN
     PATA ITITLE(1,47)/SOHFIG
     CNEL 10000 SEC. /
                                . RA JEF # 20 (JNOXIDIZED) 0.6 KEV/CHAN
     DATA ITITLE(1,48)/60HFTG
     CNEL 10000 SEC. /
                                . RA JEF # 20 (JNOXIDIZED) 0.6 KEV/CHAN
     DATA ITITLE(1,49)/60HFIG
     CNEL 10000 SEC. /
                                . RA JEF # 21 (JNOXIDIZED) 0.6 KEV/CHAN
     DATA ITITLE(1,50)/60HFIG
     CNEL 40000 SEC. /
     DATA ITITLE(1,51)/60HFIG
                                . RA JEF # 21 (JNOXIDIZED) 0.6 KEV/CHAN
     CNEL 40000 SEC. /
                                . AM 241
                                           ORTES 1/21/69
                                                           0.6 KEV/CHAN
     DATA ITITLE(1,52)/60HFIG
     CNEL 10000 SEC. /
     DATA ITITLE(1,53)/60HFIG
                                . AM 241
                                           ORTED 1/21/69
                                                           0.6 KEV/CHAN
     CNEL 10000 SEC. /
                                           ORTEC 1/21/69
                                                           0.6 KEV/CHAN
     DATA ITITLE(1,54)/6JHFIG
                                . AM 241
     CNEL 10000 SEC. /
                                           ORTES 1/21/69
                                                           0.6 KEV/CHAN
     DATA ITITLE(1,55)/63HFIG
                                . AM 2+1
     CNEL 10000 SEC. /
     DATA ITITLE(1,56)/60HFTG
                                . RA JEF # 15 (JNOXIDIZED) UNBIASED RUN
     C 40,000 SEC. /
     DATA ITITLE(1,57)/69HFIG
                                . RA JEF # 15 (JNOXÍDIZED) UNBIASED RUN
     C 40,000 SFC. /
                                . RA JEF # 15 (JNOXIDIZED) 0.6 KEV/CHAN
     DATA ITITLE(1,58)/63HFIG
     CNEL . 0000 SEC. /
                                . RA DEF # 15 (JNOXIDIZED) 0.6 KEV/CHAN
      DATA ITITLE(1,59)/EDHFIG
     CNEL 40000 SEC. /
     DATA ITITLE (1,60) /60HFIG
                                . RA JEF # 14 (UNOXIDIZED) 0.6 KEV/CHAN
     CNEL 4 CODU SEC. /
     DATA ITITLE(1,61)/61HFIG
                                . RA DEF # 1+ (JNOXIDIZED) 0.6 KEV/CHAN
     CNEL 40,000 SEC./
                                . RA DEF # 13 (UNOXIDIZED) 0.6 KEV/CHAN
      DATA ITITLE(1,52)/6)HFIG
     CHEL . 0,000 SEC./
     DATA ITTILE(1,63)/60HFIG
                                . RA DEF # 13 (JNOXTDIZED) 0.6 KEV/CHAN
     CNEL 40,000 SEC./
```

PRUGRAM SPECTRE (INPUT, OUTPUT, PLOT, TAPE1)

DATA ITITLE(1,54)/60HFIG . RA DEF # 12 (JNOXIDIZED) 0.6 KEV/CHAN CNEL ' 0,000 SEC./ DATA ITITLE(1,65)/504FIG . RA JEF # 12 (JNOXIDIZED) 0.6 KEV/CHAN CNEL 40,000 SE3./ . RA DEF # 11 (JNOXIDIZED) 0.6 KEV/CHAN DATA ITITLE(1,35)/30HFIG CNEL + 0,000 SEC./ DATA ITITLE(1,67)/50HFIG . PA JEF # 11 (JNOXIDIZED) 0.6 KEV/CHAN CNEL 10,000 SEC./ . RA JEF # 15 (JNOXIDIZED) 0.6 KEV/CHAN DATA ITITLE(1,58)/50HFIG CNEL 40,000 SEC./ DATA ITITLE(1,69)/60HFIG . RA JEF # 15 (JNOXIDIZED) 0.6 KEV/CHAN CNEL 40,000 SEC ./ DATA ITITLE(1,70)/50HFIG . AM 241 ORTED 1/21/69 0.6 KEV/CHAN CNEL 10,000 SE3./ DATA ITITLE(1,71)/50HFIG . AM 2+1 ORTED 1/21/69 0.6 KEV/CHAN CNEL 10,000 SED./ . PU 240#2 ARMINI 77 DATA ITITLE(1,72)/634FIG 0.6 KEV/CHAN CNEL 10, JOG SEC . / 0.6 KEV/CHAN DATA ITITLE(1,73)/60HFIG . PU 240 # 2 ARMANI 77 CNEL 10,000 SEC./ DATA ITITLE(1,74)/604FIG 0.6 KEV/CHAN . PU 240 # 1 ARMANI 77 CNEL 20,000 SEC./ APMANI 77 0.6 KEV/CHAN . PU 240 # 1 DATA ITITLE(1,75)/604FIG CNEL 20,000 SEC./ RA 757 # 10 (DXIDIZED) 0.6 KEV/CHANN DATA ITITLE(1,73)/60HFJG CEL 40,000 SEC. / DATA ITITLE(1,77)/504FIG RA DEF # 10 (DXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / DATA ITITLE(1,78)/604FIG RA 757 # 11 (DXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / DATA ITITLE (1,79) / 60HFIG RA DE= # 11 (CAXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / RA 7== # 12 DATA ITITLE(1,80)/30HFIG (DXIDIZED) 0.6 KEV/CHANN CEL 46,000 SEC. / DATA ITITLE(1,81)/60HFIG RA DEF # 12 (DXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / DATA ITITLE (1,82) / 60 HFIG RA 7== # 13 (DXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / RA DEF # 13 (OXIDIZED) 0.6 KEV/CHANN DATA ITITLE(1,83)/60HFIG CEL 40,000 SEC. / RA 7== # 14 (OXIDIZED) 0.6 KEV/CHANY DATA ITITLE(1,84)/60HFIG CEL 40,000 SEC. / DATA ITITLE(1,85)/304FIG RA DEF # 14 (DXIDIZED) 0.5 KEV/CHANN CFL 40,000 SEC. / DATA ITITLE(1,85)/30HFIG RA 75 # 15 (DXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / RA 7== # 15 DATA ITITLE (1,87)/50HFIG (DXIDIZED) 0.6 KEV/CHANN CEL 40,000 SEC. / RA 75 # 16 ()XIDI 7ED) 0.6 KEV/CHANN DATA ITITLE(1,83)/504FIG CEL 40,000 SEC. / RA DEF # 16 DATA ITITLE (1,83)/50HFIG (DXIDIZED) 0.5 KEV/CHANN CFL 40,000 SEC. / . AM 241 (ORTED) UNBIASED RUN DATA ITITLE(1,90)/50HFIG 0.6 KEV/C CHANNEL 10 KSEC ./ DATA ITITLE(1,91)/50HFIG . AM 241 (ORTES) UNBIASED RUN CHANNEL 10 KSEC . / . BACKGROUND COUNT (BIASED) DATA ITITLE(1,92)/604FIG 40000 SEC

```
DATA ITITLE(1,93)/604FIG
                                  . BACKGROUND COUNT (PIASED)
     C.
C THE FIRST SPECTRUM TO BE PLOTTED MUST BE REGISTERED BY THE USE OF THE
C SKIPF CONTROL CARD
C
              NTAG (1,N) IS THE TAGWORD TO BE PLOTTED
C
               NTAG(4, N) IS THE LAST CHANNEL TO BE PLOTTED
C
               NTAG(3,N) IS THE FIRST CHANNEL TO BE PLOTTED
C
              NTAG(2,N) IS THE TYPE OF PLOT:
                                                   1 = SMALL FOR PUBLICATION
                                                   2 = LARGE
C
C
      PEAD , YA (1), XA (1), YA (2), XA(2)
      FIRST, THE TAGWORDS TO BE PLOTTED AND OTHER DATA (NTAG)
C
      ARE FEAD
C
C
      J= U
    5 J=J+1
      READ', (NTAG(I, J), I=1, 4)
      IF (NTAG (1, J) .GT. () GO TO 5
      PRINT'," TAGWORDS ", (NTAG(1, JJ), JJ=1, J), " TO BE PLOTTED "
      CALL ARYODR (NTAG, J)
      N = J
      DO 900 I=1.N
      XAXIS=XA(NTAG(2,I))
      YAXIS=YA(NTAG(2,1))
      APLE = XAXIS + 4.0
      K = NT + G(4, I) - NT + G(3, I) + 1
C BEGIN WOFKING ON SPECTRA
   11 NN=1
      KK=1
C READ IN THE Y VECTOR
      BUFFER IN(1,0) (MW(1), MW(160))
 40
      KK=U! IT(1)
      CALL EPRSET (KOUNT, 100)
 50
      DECODE (150,60, MW) M, 44,7
      FORMAT (2X, 14, 2X, 44, 23FE. 0, 3 (/25F3. 0), /,8F5. 0)
 50
      PRINT*," TAGWORD NUMBER ",M," READ "
      IF (M -NTAG(1,I)) 11,70,900
   70 CONTINUE
     · IF (KCUNT.GT.0) GO T) 190
   71 CONTINUE
      DO 100 J=1,256
      Y(NN) = 7(J)
 100
     NN=NN+1
      IF (KK.NE.0) GO TO 40
C SET UP THE X VECTOR
      X(1) = FLOAT(NTAG(3,I))
      00 10 II=2.K
   10 X(II)=X(II-1)+1.0
      X(K+1) = X(1)
      X(K+2) = FLOAT(K)/X4XIS
```

```
C EPPOR EDIT SEE PROGREM SCRIPT
IF IE EQUALS ZERO THAN THERE ARE ERRORS IN THE Y VECTOR FROM SCRIPT
 C NE IS THE NUMBER OF ERRORS IN THE VECTOR Y
       FEAD 1000, IE, NE
       IF (IE.EQ. 0) GO TO 300
 C SET UP PLOTTER
       CALL PLOT (0.0, -3.0, -3)
       IF (NTAG(2, I) .GT .1) GO TO 20
       CALL PLOT (1.0, 3.0, 3)
       CALL PLOT (1.0,8.6,2)
       CALL PLOT (4.0, 9.5, 3)
       CALL PLOT (9.0,9.5,2)
       CALL PLOT (12.0,8.0,3)
       CALL PLOT (12.0, 3.0, 2)
       CALL PLOT (9.0, 1.0, 3)
       CALL FLOT (4.0, 1.0, 2)
       CALL PLOT (2.25, 2.0, 3)
       CALL PLOT (2.25,8.0,2)
       CALL PLOT (11.0,3.0,2)
       CALL FLOT (11.0, 2.0, 2)
       CALL PLUT (2.25, 2.0,2)
       CALL PLOT (2.75,2.5,-3)
       GO TC 21
   190 PRINT+," BAD DATA READ, TAGWORD # ", M
       GO TO 71
    20 CALL PLOT (1.0, 2.0, -3)
    21 CONTINUE
 C
 C SCALE Y VECTOR
  200 DC 210 J=1,K
   210 Y(J) = Y(J+NTAG(3,I)+NOFF-1)
       T=8=Y(1)
       DO 220 J=1,K
       IF(Y(J) \cdot GT \cdot T)T = Y(J)
       IF(Y(J).LT.S)3=Y(J)
  220
      CONTINUE
       Y (K+1)=B
       Y(K+2) = (T-B) /YAXIS
 C PLOT RESULTS
       CALL AXIS(0.0,0.0,74CHANNEL,-7, YAXIS, 0.0, X(K+1), X(K+2))
       CALL AXIS (0.0,0.0,6400UNTS,6,YAXIS, 90.0,Y(<+1),Y(K+2))
       CALL LINE (X, Y, K, 1, 0, 1)
       PRINT 1030, M
       CALL SYMBOL (1.0, SYM, 0.105, ITITLE(1, 4), 0.0, 50)
       CALL PLOT (ASLE, 0.0, -3)
  300
       CONTINUE
       CALL PLOTE
       STOP
       DO 316 J= 1.NE
       READ 1010.IC.AC
       IC=IC+1
```

```
310 Y(IC)=AC

GO TO 200

1000 FORMAT(2I5)

1010 FORMAT(I5,F10.0)

1020 FORMAT(2F10.0)

1030 FORMAT(1X,"TAGWORD PLOTTED",T18,[5)

END
```

SUBROUTINE ARYOTP (NARRAY, N)
DIMENSION MARRAY(+, N), ISAV(4)
NP=N-1
DO 50 I=1,NP
K=I+1
DO 50 J=K,N
IF (NARRAY(1,I) .LE.NAPRAY(1,J)) G) T) 50
DO 30 M=1,4
ISAV(M) = NARRAY(M,I)
NARRAY(M,I) = NARRAY(M,J)
30 NARRAY(M,J) = ISAV(M)
50 CONTINUE
RETURN
END

SUBPOUTINE HALVE(SPEC, FWHM, RWHM) REAL LWHM, RWHM DIMENSION SPEC (2100) PKMAX=1J0. DO 100 I=10,2100 IF (SPEC(I) . LE. PKMAX) GO TO 100 PKNAX=SPEC(I) IPEAK=I 100 CONTINUE HAFMAX=PKMAX/2. J=IPEAK 150 J=J+1 200 IF (SFEC(J).GT.HAFMAX) GO TO 150 RWHM=J+(SPEC(J)-HAFMAX)/(SPEC(J-1)-SREC(J)) J=IPEAK 250 J=J-1 IF (SFEC (J) . GT. HAFMAY) GO TO 250 LWHM=J+(HAFMAX-SPEC(J))/(SPEC(J+1)-SPEC(J)) FWHM = RWHM-LWHM PRINT*," PKMAY = ", PKMAY," LWHM = ", LWHM, " FWHM = ", FWHM," RWHM= " C, RWHI RETURN END

Appendix E

User Instructions for SPECTRE

Program SPECTRE is designed to allow the user to select the tagword to be plotted, choose a large or small format, and select the range of channels for the plot with one card for each spectrum to be plotted. A set of title statements are initialized by the use of DATA statements.

The file containing the spectra to be read must be placed on file TAPE1 as for Program SCRIPT, but the first spectrum need not be registered. It is more efficient to advance the file pointer to just before the smallest tagword to be plotted, but this is not absolutely necessary.

A series of 2N+1 data cards are required to plot N spectra. The first card must have the axial dimensions in inches for the two plot formats in the following order: counts (small), channel (small), counts (large), channel (large). These are normally 5.0, 7.0, 8.0, 12.0. In the large format, the counts axis is limited by the width of the plotter to less than nine inches but the channel axis is unlimited. The small format dimensions should not be changed.

Next should come a series of cards with the information for each spectrum to be plotted. Each card should contain in order the tagword to be plotted, the type of plot (1 = small, 2 = large), and the first and

last channels to be plotted.

Finally, error data cards are added for each spectrum to be plotted. Each card should contain IE and NE in 215 format with

IE = Is there an error?

0 = Yes

Not 0 = No

NE = Number of errors

If IE = 0 there should be NE cards containing the channel number and new value for each error in format I5, F10.0. These will be read before the next error data card.

The order of the tagword cards is unimportant since they will be placed in sequence from smallest to largest by subroutine ARYODR.

However the error edit cards must be in correct sequence to match the tagwords after the tagwords are ordered by ARYODR.

The SCOPE control cards required are similar to those for SCRIPT.

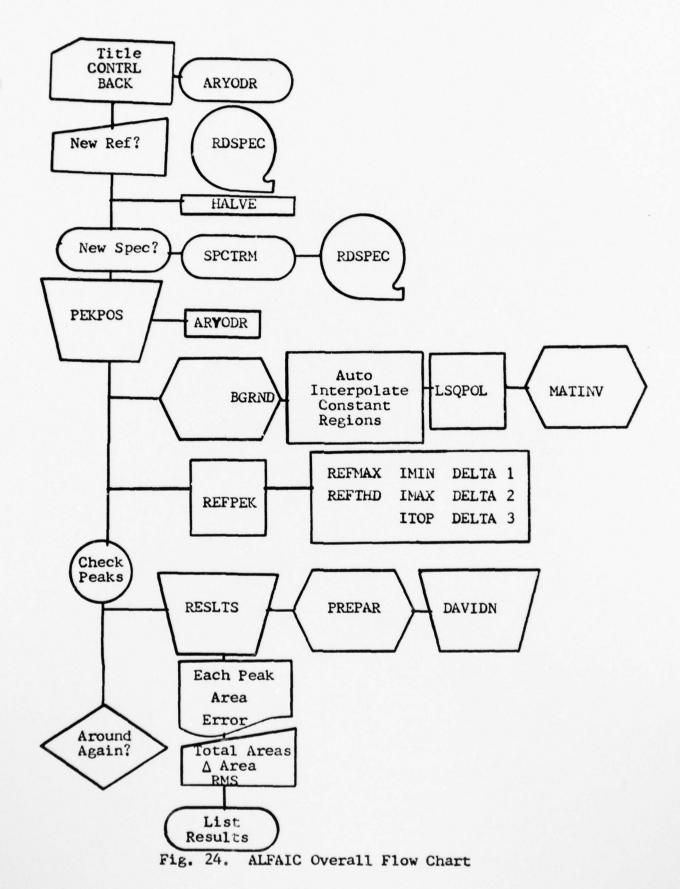
Appendix F

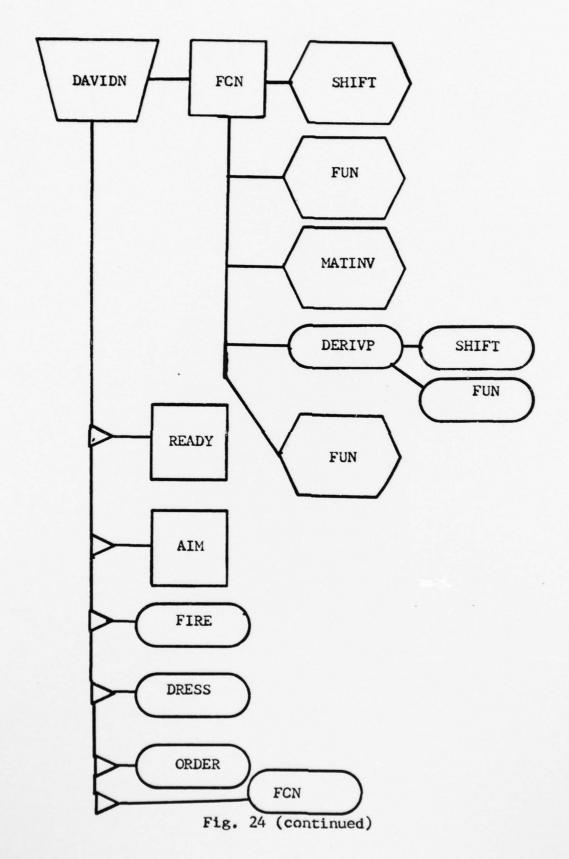
Overview of Program ALFAIC

This appendix is a discussion of the general flow of action in program ALFAIC. Refer to the block diagram in Figure 24.

The main program first reads certain controlling data including the run TITLE card, NAMELIST CONTRL, and the background values BACK, which are then sent to ARYODR to be placed in correct sequence. The program then calls RDSPEC to read in a reference spectrum from file TAPE1. Subroutine HALVE computes the FWHM for this spectrum. The program then calls SPCTRM, which in turn calls RDSPEC to read the spectrum to be analyzed. Then the tentative positions of peaks to be resolved are read into PEKPOS and sent to ARYODR for ordering. On subsequent iterations, the program will read in a specified number of reference spectra to use to analyze this same unknown.

Now the program calls BGRND, which can perform one of three options. BGRND can automatically compute the background using subroutines LSQPOL and MATINV. It can also compute an interpolated background function through a designated set of points. The third option, which was used throughout this study, is to compute a number of regions of





constant background from data in BACK.

Next, the program calls REFPEK which computes certain parameters for the reference peak. These may instead be specified and the program will compute a reference to match or the program can compute a reference from the spectrum to be analyzed. The parameters are based on the highest and lowest nonzero values in the reference spectrum, the maximum value in the reference peak and the one-third maximum point to the right of the peak.

The program then checks the peaks to determine if they can be fitted within the range of the spectrum using a reference peak of the length computed in REFPEK.

Finally, the program calls RESLTS, which passes the data on to PREPAR. When the computed spectrum is returned from PREPAR, RESLTS computes the areas and estimated errors for each peak and the total areas of both the unknown and the resolved or calculate spectra and the square root of the sum of the square of the difference between these two spectra at each point.

PREPAR sets up the problem for DAVIDN, which calls FCN and then, as required, calls READY, AIM, FIRE, DRESS, ORDER, and FCN again. FCN utilizes SHIFT, FUN, MATINV, and DERIVP to help it search for the minimum Chi-Squared Function. These routines collectively do the work of calculating a spectrum which is the result of a constant for each peak multiplied by the reference spectrum at each point relative to that peak location. These individual components are then added to give the combined spectrum.

Appendix G

Input Cards for ALFAIC

Introduction

ALFAIC allows the user a plethora of options, but placing the input cards in the correct order is critical if the program is to function as desired. The program can be run in two main ways, analyzing real data or internally generated data.

Conjur Option Conversion

As listed, the program analyzes real data from file TAPE1 and the routines CONJUR, FACTOR, PPOISS, PGAUSS, and OUTPUT are not used. By replacing the calls to RDSPEC with calls to CONJUR, the program may be converted to analyzing randomized Gaussian spectra. Input 6 should be substituted for Input 5 if this version is used.

Standard Version

The unknown spectrum and NRSPEC reference spectra should be placed in file TAPE1 in the following order:

Reference spectrum 1

Unknown spectrum

Reference spectra 2- NRSPEC

FILE and LDSET control cards are needed as for Programs SCRIPT

and SPECTRE.

Input Cards

Input 1. Title Card

FORMAT (8A10)

The title for this complete sequence is read from the first card. End of file or blank terminates the run.

Input 2. NAMELIST CONTRL

= -n

NBACK = 0 Background determined automatically by program.

Background option I. The X and Y coordinates for n background points will be read in i program calculates a curve passing

through all points.

Background option II. n background intervals will be read in (background is a constant between the limits of each interval).

Note 1: $|n| \le 50$ If n > 50, the program will truncate it to 50.

Note 2: n ≥ 3 for background Option I (positive sign).

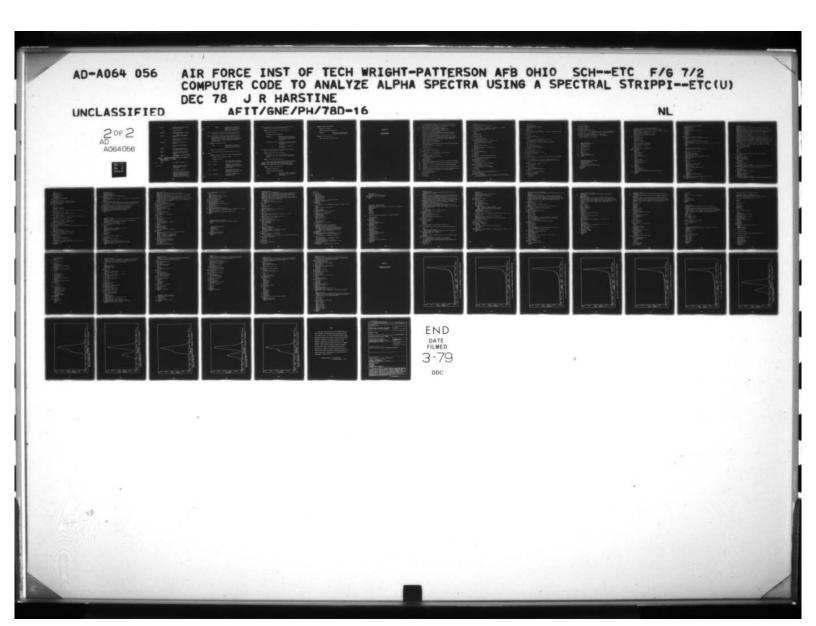
NPKRD ≥ +1 Initial peak positions to be read, as values of channel number.

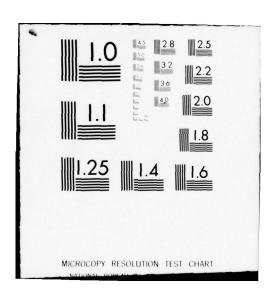
NREF = 0 Reference peak to be selected from the spectrum. (This option is generally not recommended.)

= -1 Reference peak spectrum to be read from tape.

NSSW1 = 1 Print the results from variablemetric-minimization routines.

= 0 Suppress the above.





List the raw data, resolved peaks, NSSW2 = 1and composite spectra. = 0Suppress the above. The maximum number of channels MAXREF = in the reference peaks. KEPREF = 0 Read in NRSPEC new reference spectra. Use the reference spectra from = 1 the last analysis. KEPDAT = 0 Read in a new spectrum to be analyzed. = 1 Analyze the last data spectrum again. STDEV = ' The standard deviation of the Gaussian spectra to be analyzed. STDEL = The amount the different reference spectra are varied around STDEV. The number of reference spectra NRSPEC = to be used.

Input 3. Background Data Cards (not used for NBACK=0).
DB(I), BACK(I), I = 1, NBACK
FORMAT (16F5.0)

1-5 DB(I) =

For NBACK > 0 (option I).

11-15, etc.

DB(I) is the channel number at which a background value is to be specified.

For NBACK < 0 (option II):

DB(I) is the channel number at the lower end of the Ith interval for which a background value is to be specified. DB(1) is supplied by the program and may be left blank.

6-10 BACK(I) =

The value of the background for the Ith background position (NBACK > 0), or for the Ith background interval (NBACK < 0).

- Note 1: The pairs DB(I), BACK(I) may be given in any order. The program will rearrange them in increasing order of DB(I).
- Note 2: For NBACK > 0, the program requires backgrounds for the first and last channels of data. If not given explicitly, the program will use BACK(1) for the first channel, and BACK (NBACK) for the last channel. These program-supplied values may be counted for meeting the minimum requirement of 3 background points.

Input 4. Peak extraction channel

IPK =

The desired channel number of the maximum count in the 512 channel segment to be analyzed.

Input 5. DO Loop Sequential data

Five sequences of these cards will be required for each analysis.

Input 5a. Reference Peak Parameter Card (Use only if NREP=0.)

STOIPR, DELTA1, DELTA2, DELTA3

FORMAT (4F10.5)

1-10	STOIPR =	The channel number of the maxi- mum count in the reference peak.
11-20	DELTA1 =	Channels from the front (high- energy) edge of the reference peak to the "third-height" position on the front edge.
21-30	DELTA2 =	Channels from the back (low- energy) edge of the reference peak to the third-height position.
31-40	DELTA3 =	Channels from STOIPR to the third-height position.

Note: For MCA operation, the "third-height" position is defined as STOIPR and hence the program sets DELTA3=0.0.

Input 5b. Peak Position Cards (Use with NPKRD > +1.)

PEKPOS(I), IFIXPK(I)

UNFORMATTED (LIST DIRECTED)

PEKPOS(I) = The estimated third-height location of the Ith peak to be considered by the program, specified in chan-

nel number.

IF1XPK(I) = 0 or blank The program will adjust PEKPOS(I)

for the best fit to the data. (Stand-

ard option.)

>i PEKPOS(I) will be held fixed by

the program.

Note: The cards may be in any order. The program will rearrange them into ascending order of PEKPOS(I).

Input 5c. Peak Position Termination Card

PEKPOS(I) < -1.0. This will terminate peak locations and the program will process a new set of data, beginning with Card 1.

Input 6. Conjured Data Sequence Cards

These are used instead of INPUT5 when running the program using data to be created by Subroutine CONJUR and the associated functions. The two statements in ALFAIC and SPCTRM calling RDSPEC must be replaced with calls to CONJUR for these options.

Input 6a. Channels of desired peak(s)

IPEAK(N), N=1, NPEAK

UNFORMATTED (LIST DIRECTED)

IPEAK =

The center channel of the Gaussian peak to be created by calling function PGAUSS.

Input 6b. Heights of desired peaks

IHITE(N), N=1, NPEAK

UNFORMATTED (LIST DIRECTED)

IHITE(N) =

The approximate height in counts of the peak in channel IPEAK(N).

Input 6c. Peak position cards

These are the same as Inputs 5b and 5c.

Appendix H

Program ALFAIC

```
PROGRAM ALFAIC(INPUT, OUTPUT, TAPE;=[NPUT, TAPE6=OUTPUT, PUNCH,
        TAPE7=PUNCH, TAPE9, FAPE1)
      FRUGEAM ALPHAFIT WAS OPPIATED FOR PARTIET WRITTEN BY
C
C
      J.R. COMFORT OF ARGONNE NATIONAL _430RATORY
      THIS PROGRAM ALLOYS THE FOLLOWING:
C
C
      A MAXIMUM OF 2100 CHANNELS FOR A REFERENCE PEAK
C
      A MAXIMUM OF 2101 CHANNELS FOR A SPECTRUM
C
      A MAXIMUM OF 50 CHAINELS FOR A PICKGROUND INPUT
      COMMON /A00/ VM1(582), MSSW1, NSSW2
      COMMON /AG2/ DUMANS(161), STORV1(2100), RAAX(2100), ITIMES, NNX
      COMMON/AS3/ TITLE(21), PEKPOS (20), IFIXPK(20), BETA, GSTATE,
     1 GSOVAL, NT, NOALC, ICS, LO
      COMMON /A0+/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
        STOIPR, REFYAX, IT1, ID2, IDT, N3, NE, NREF
      COMM(N /A05/ 3ACK2(2100), 08(50), 3ACK(50), NJ, NBACK, NPKRD
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FRED, OFTEN,
       NOFTEN, NOHAMM, II, TJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
      COMMON /OPTN/ KEPREF, KEPDAT
      DIMENSION REF3TO(2100,10), FWHM(10,2)
      EQUIVALENCE (IBLNK, 3LNK, DSLNK)
      DATA (DALNK=8H
      NAMELIST/CONTRL/NBACK, NPKRD, NREF, NSSW1, NSSW2, MAXREF, KEPREF, KEPDAT
     C.STDEV, STDEL, NRSPEC
         ... START CALCOMP AND GET DATE ...
C
      IEKR = 0
       GALL DATE (TODAY)
      GO TC 50
         ... TERMINATE PROGRAM ...
      WRITE (6, 101)
  101 FORMAT (3X.18H ENDPLOT EXECUTED)
         ... READ AND WRITE TITLE CARD. EXIT ON E.O.F...
C
   50 PEAD(5,10)
                         (TITLE(I), I=1,3)
       IF(EOF(5)) 45,49
   49 IF (TITLE(1).ED.BLNK) GO TO 45
      WRITE(6,30) (FITLE(I), I=1,8 ), TODAY
C
         ... INPUT OF DATA ...
      FEAD (5, CONTPL)
      IF (EOF (5)) 45.51
   51 PRINT CONTRL
      KEPREF IS AN OPTION TO ALLOW THE JSER TO KEEP THE SAME REFERENCE
C
      PEAK FOR ALL ANALYSIS
C
      KEPREF.GT.O ALLOWS THE USE OF THE SAME REFERENCE PEAK FOR ENTIRE
C
      ANALYSIS
      KEPREF.EQ.J REQUIRES A NEW REFERENCE PEAK WITH EACH SPECTRUM
C
C
      ANALYZED
C
      KEFOAT IS AN OPTION TO ALLOW THE SAME DATA SET TO BE USED FOR ALL
C
      ANALYSIS.
C
      MEPDAT .GT.O ALLOWS THE SAME DATA SET TO BE USED FOR THE ANALYSIS.
      KEPDAT . EQ. O RETUIRES A NEW DATA SET FOR EACH ANALYSIS.
      MAXP2 = MAXREF + 2
      IF (NREF.GT.10) NREF = 10
      IF (NBACK) 76,196,87
   70 NJ = -1194CK
      NAVCK = 5
      GO TO 90
   80 NJ = NPACK
```

```
NACK = 1
   90 IF (NJ.GT.50) NJ = 30
      READ(5,14) (03(I), 340K(I), I=1,NI)
      00 91 I=1.NJ
   91 PRINT*," 93(",I,") = ",93(I)," 310K(",I,") = ",BACK(I)
      IF (NJ.GT.1) GALL ARYONR (OR, RACK, NJ, 2)
         ...INITIALIZATION ...
  100 CONTINUE
      LO=0
      NADJ=0
      STOIFR = 0.0
      00 165 I=1,20
  105 \text{ JFIXPK(I)} = 0
      DO 110 I=1, MAXREF
  110 STOREF(I) = 0.0
C
         ... MORE DATA INPIT ...
      IF (NRSF) 120,130,150
  120 IF (KEFREF.GT.3)G0 TO 778
      PRINT .. " CALLING ROSPEC FOR REFERENCE PERK "
      GO 1001 TUK=1, NRSPEC
      CALL ROSPEC (STOREF, N, NTAG, MAXREF)
      MSTOK = N
      00 77 I =1.N
      REFSTO(I.IJK)=STOREF(I)
  77 CONTINUE
      CALL HALVE(REFSTO(1, IJK), FWHM(IJ(,1))
      FWHM(IJK,2) = IJC
 1001 CONTINUE
      GO 70 1000
      DO 99 I = 1, NSTOR
 778
      STOREF(I) = REFSTO(I, IJK)
   99 CONTINUE
 1000 CONTINUE
      GO TO 150
  130 READ (5,18) STOIPR, DELTA1, DELTA2, JELFA3
  15G CONTINUE
         ... GET A STANDARD SPECTRUM DATA SET ...
      IF (KEPDAT.GT.0) GO TO 175
  170 CALL SPOTRM
  175 IF (JERR.GT.0) GO TO 45
      WRITE (6, 34) NCHANN
      DELTA3 = 0.0
         ... READ PEAK POSITIONS, DISTANCE
  200 00 220 I=1,21
  210 PEAD , PEKPOS (I), IFIYPK (I)
      IF (FEKPUS(I).LE.-1.) GO TO 230
       PRINT*," PEAK# ",I," = ",PEKPOS([)
  220 CONTINUE
      95 = TM
      GO TC 240
  230 NT = I - 1
  240 IF (NT.GT.1) CALL ARYOTR (PEKPOS, IFIXPK, NT, 2)
      IPK1=PEKFOS(1)
  330 DO 3! 0 I=1,NOHANN
  350 PAWX(I) = COUNTS(I)
          ...CALC. PACKGROUND, SELECT REFERENCE PEAK AND PICK PEAKS...
      CALL HALVE (RAWX, FWHM1)
```

```
DIFMIN = 50.
      DO 300 I=1.NRSPEC
      DIFF=APS(FWHM1-FWHM(I,1))
      IF (DIFF.GT.DIFMIN) GO TO 300
      DIFMIN=DIFF
      IJK=I
  300 CONTINUE
      JF (DJFMIN.LT.50.) G7 TG 301
      PRINT " UNSATISFACTORY REFERENCES, FWHY OF UNKNOWN IS ", FWHM1,
     C" CHANNELS "
      GO TO 10
  301 CONTINUE
      DO 3L2 I=1. NSTOR
      STOREF(I) = REFSTO(I,IJK)
  302 CONTINUE
      114X = 0
      IF ((NBACK.E0.0).4ND. (NPKRD.E0.01) 30 TO 4+0
      IF (NMACK.EQ.0) 30 TO 370
      IF (PB(1).LT.DIST(1)) PB(1) = DIST(1)
      IF (DB(NJ).GT.DIFT(NCHANN)) DB(NJ) = DIST(NCHANN)
  370 CALL PERN:
      NNX = NNX + 1
      00 420 I= : . NCHANN
      IF (FANX.I)) +20,+20,410
  410 FAWX (I) = AWX (I) -84 CK2 (I)
      IF(RAWX(I) \cdot LT \cdot 0 \cdot C) \quad RAWX(I) = 0 \cdot 0
  420 CONTINUE
  440 CALL REFFEK
      IF (NPK ( NE. 0) GO TO FOR
  460 DO 470 I=1.NT
  470 PEKPOS(I) = PEKPOS(I) + DELTA3
      IF (MNX) 370,370,523
  500 WRITE( ,, 38)
      GO TC 3:3
  520 WRITE (3.40)
      ... PAKE SURE THAT ALL PEAKS ARE IN THE RANGE OF THE SPECTRUM
C
  530 H = 1
      00 550 I=1.NT
      IF (()*KFOS(I) -DELTA2-2.*OFTEN)..T.DIST(1)) GO TO 550
      IF (('EKPOS(I)+DELTA1+2.*OFTEN).JT.DIST(NDHANN)) GO TO 550
      M = M + 1
  550 CONTINE
      PRINT'," NADJ = ",NADJ," Y = ", Y
      IF (M.(E.NT) GO TO 580
      DO 560 I=1,50
  560 STORFF(I) = U. 0
      NADJ = NADJ+1
      IF (NAD. LT.10) GO TO 440
      PRINT", " UNSATISFACTORY PEAKS"
  580 NT = 1
      PRITE(f,42) (PEKPOS(I), I=1, NT)
      DO ELI I=1.1 CHANY
  600 STORV!(1) : BACK2(1)
      CALL FESLTS
      KEPOA" =1
      CO T 1 50
```

```
10 FOR 1 T( A10)
12 FORMA" ( 14,412,14
14 FORMA! (11 F5.0)
16 FORMAT(I! . 15F5.3)
18 FORMAT : 4F10.5)
24 FORMAT (F9.4, I1, F10.3)
30 FORMAT(1H1, 1X, 8410, 10Y, A10)
32 FORMAT (10HO
                            4X8HNBACK = I4,4X3 HNPKRD = I2,4X7HNREF = I2
                     4 X3 HNSSW1 = I2, + X3 HNSSW2 = I2, 4 X9 HMAXREF = I4)
  1,4X9H
34 FORMAT (11HO NCHANN = I5,5X7H
38 FORMAT (35HO INITIAL SUFSSES OF PEAK POSITIONS)
40 FORMA (LUHO CALCULATED ESTIMATES OF PEAK POSITIONS)
42 FORMA (10F12.3)
44 FORMAT (1HO, I4, 14H PEAKS DELETED)
   END
```

FUNCTION FACTOR(N) DOUBLE PRECISION FI, SUM FACTOR = 1. 11 IF(N-1)40,40,13 13 IF (N-10) 21, 21, 31 21 00 23 I=2,N FI=I 23 FACTOR=FACTOR*FI GO TC 40 SUM= (. 31 00 34 I=11, N FI=I SUM=SUM+DLOG (FI) 34 35 FACTOR=3628800.*DEX7(SUM) 40 RETURN END

```
SUBROUTINE CONJUR (SPEC, NPEAK, STDEV, NCHANN)
      DIMENSION SPEC (4000), DIST (4000), POIST (200), IPEAK (5)
      DIMENSION IHITE(!)
      PRINT+, " NPEAK = ", NPEAK, " STDEV = ", STDEV, " NCHANN = ", NCHANN
      READ*, (IPEAK(N), N=1, NPFAK)
      PRINT+," IPEAK = ", (IPFAK(N), N=1, NPEAK)
      READ*, (IHITE (N), N=1, NPFAK)
      PRINT+," IHITE = ", (IHITE(N), N=1, NPEAK)
      00 100 I=1, NCHANN
100
      SPEC(I)=0.0
      00 1000 J=1, NPEAK
       AVERAG=IFEAK(J)
      SIGMA = STDEV
      A=37.878 * IHITE(J)
      00 200 I=1, NCHA'N
      X = I
      SPECTR=A+PGAUSS(X, AVERAG, SIGMA)
      IF( ] .LT. AVERAG ) GO TO 101
      IF (SFECTR.GE. 0.1) GO TO 101
      SPECTE = 0.0
      GO TC 102
  101 IF (SPECTR.LT. 1.0) SPECTR = 1.0
  102 SPEC(I) = SPEC(I) + SPECTR
200
       CONTINUE
1000
      CONTINUE
      NSEET = 2001
      CALL RANSET (NSEED)
      AVERAG = 20.
      IMAX= 2* AVERAG
      DO 400 I=1. IMAX
4.00
      DIST(I)=PPOISS(I, AVERAG)
      IOLD=1
      NP=0
      DO 500 L=1, IMAX
      A=DIST(L) *IMAX
      IF(A.LT. 1.0) GO TO 500
      INFW=IOLD+4
      DO 450 J1=IOLD, INEW
      PDIST(J1) = L
      NP=NF+1
      CONTINUE
450
      IOLD= INEW+1
500
      CONTINUE
      DO 6CC I=1, NCHANY
      IJ=RANF(N)+NF
      IF(IJ.LT.1) GO TO 600
      SPEC(I)=SPEC(I)+SORT(SPEC(I))+(P)IST(IJ)/AVERAG-1.0)
600
      CONTINUE
      RETURN
      END
```

```
SUBROUTINE HALVE (SPEC, FWHM, RWHM)
     REAL LWHM, RWFM
     DIMENSION SPEC (2100)
     PKMAX=100.
     CO 100 I=10,2100
     IF (SFEC (I) . LE.PK MAX) GO TO 100
     PKMAX=SPEC(I)
     IPEAK=I
100 CONTINUE
     HAFMAX=PKMAX/2.
     J=IPEAK
 1-0 J=J+1
 200 IF (SPEC(J). GT. HAFMAY) GO TO 150
     RWHM=J+(SPEC(J)-H4F44X)/(SPEC(J-1)-SPEC(J))
     J=IPFAK
 250 J=J-1
     IF (SFEC (J) . GT . HA = 14 Y) GO TO 250
     LWHM=J+(HAFMAX-SPEC(J))/(SPEC(J+1)-SPEC(J))
     FWHM = RWHM-LWHM
     PRINT+," PKMAX = ", PKMAX," LWHM = ", LWHM, " FWHM = ", FWHM, " RWHM= "
    C.RWHM
     RETURN
     END
     SUBROUTINE RESPEC(Y, N, M, MAX)
     DIMENSION Y (4100), X (256), MW (160), Z (320)
     N=1
     KK=1
  10 BUFFER 1N(1,0) (MW(1), MW(160))
     KK=UNIT(1)
     CALL EPRSET (KOUNT, 100)
     DECODE (150, 6 C, MW) 4, 4M, X
     IF (KOUNT.GT.0) GO TO 10
  50 FORMAT(2X,14,2X,14,23F6.0,9(/25F5.0),/,8F5.0)
     IF (KK.EQ.0) GO TO 81
     DO 80 I=1,255
     Y(N) = X(I)
  90 N=N+1
     IF (KK.NE.0) GO TO 10
  31 N=N-1
     ITIME=Y(1)
     IF (ITIME.ER. 0) ITIME =40000
     PRINT+," ITIME = ",ITIME
     PRINT 1010, M
     IF (N.LE.MAX) GO TO 39
     PRINT+," N GREATER THAN MAX, N= ", V
     N=MAX
  39 NN=(N/10) +1
     DO 90 K=1,NN
     IN= (K-1) + 10
     II=IN+1
     IJ=IN+10
     PRINT 1020, IN, (Y(J), J=II, IJ)
90
     CONTINUE
     RETUFN
1010 FORMAT (1HO, TE1, "TAGNORD NUMBER", 5K, 15, 5X, "READ")
1020 FORMAT(1X, 15, 10F10.0)
```

```
SUBROUTINE RESLTS
      DIMENSION FHI(6), HORD(20)
      DIMENSION PEKERR(200), PKBACK(200), XSECTS(200), XSECER(200),
     1 ORELT(200) , EX(200)
      COMMON /A00/ VMM(563), IHOLD(20), NSSW1, NSSW2
      COMMON/A01/S TORT(21)2,10),S(2102),ITSTRT(20),ITSTOP(20),DUM(5538)
      COMMON /402/ SIGM4(20), ERRZ(20), PERSTO(21), STORHH(20),
     1 XINTIS(20), INDFX(20), INITAL(20), IFINAL(20), STORV1(2100),
     2 RAWX (2100), ITIMES, MNX
      COMMON/A03/ TITLE(20), PEKPOS(20), IFIXPK(20), BETA, GSTATE,
       GSCVAL, NT, NCALC, IGS, LQ
      COMMON /A0+/ INTREF(20,10),STORFF(2100),DELTA1,DELTA2,DELTA3,
        STOIPR, REFMAX, ID1, ID2, IDT, NB, NE, NREF
      COMMON /405/ BACK2(2100), DB(50), 34CK(E0), NJ, NBACK, NPKRD
      COMMON /SATA/ DIST(2100), SOUNTS(2100), RUNID, TODAY, FREQ, OFTER,
     1 NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
      DATA(FMT=8H(1XF3.4,, 7H3F10.2,, 14 , 5HF10.2, 5H/40X,, 5H 9F10.2))
                                        3, 6H 10X, 3, 6H 20X, 7,
      DATA (WORD
                              = 84
                                    50x, +, 8H
                                                50X, 3, 3H 70X, 2,
                        40X, 5, 84
        84
            30X, 6, 8H
                              9, 8H
                                    10x, 3, 8H 20x, 7, 8H
            80X, 1, 8H
                                                             30X, 6,
       8H
            40x, 5, 3H
                                    60(, 3, 8H 70X, 2, 8H
       84
                        50X, 4, 8H
                                                              30X. 1.
     4 8H
                 9, 3H
                        19X, 8)
      DATA (ISF=1HF), (J3LNK=1H)
C
         ...INITIALITATION ...
      JQ = 0
      JOB = 0
      NNX = 1
      MTP = 1
      MTT = 1
      NT1 = NT
         ... STORE INFORMATION AND GET READY TO SALL PREPAR...
   50 DO 70 I=1,NT
      J = NNX + I - 1
      IHOLD(I) = IFIXPK(J)
   70 PERSTO(I) = PEKPOS(I)
   90 DELTA1 = DELTA1/OFTEN
      DELTA2 = DELFAZ/OFTEN
      CALL PREPAR
      DO 140 I=1,NT
      J = NNX + I - 1
  140 IFIXPK(J) = 1HOLD(I)
      NNX = NNX + NT
      IF (NSSW2.G1.0) ARITE(E,9042)
 3072 FORMAT(10H0 DISTANCE, 2X8HRAW DATA, 2X10HEACKGROUND, 2X9HCOMPOSITE, +X
     116HRESOLVED SPECTRA)
         ... CALCULATE AREAS AND ERRORS FOR THIS GROUP ...
      00 91 I=1, VT
      XINTIS(I) = 0.
      DO 3005 J=1, MAXP2
 300 = XINTIS(I) = XINTIS(I) + STORZ(J.[)
      JQ=J0+1
      PEKPOS (JO) =PERSTO (T)
      PEKEFR (JQ) =SIGM4(I)
      PKBACK(JO) = 0.0
      XSECTS(JQ) = XINTIS(I)
   31 XSECER(JO) = XSECTS(JO) ERR7(I)
         ...ADD BACKGROUNDS AND PRINT THE RESOLVED AND COMPOSITE SPECTRA
```

```
JPP = 0
     D03300 I=1, I TIMES
     MOP = JPP + 1
     JPP=MOP+INDEX(I)-1
     MZZ=INITAL (I)
     MMX=IFINAL(I)
     IF (NSSW2.E0.0) 30 TO 1530
     IF(M7Z-MIT) 2011,2011,2010
2010 MZP = MZZ - 1
     00 2012 L = MTT, 47P
2012 WRITE(6,FMT) DIST(L), COUNTS(L), 340(2(L)
2011 WRITE(6,9032) (PERSTO
                            (JP), JP=M29, JPP)
9082 FORMAT (40X, 9=10.2)
1530 DO 3010 J=427, MMX
     K1 = 0
     K2 = 0
     M = J - MZZ + 1
     STORV1(J) = BACK2(J)
     00 1310 JP = MOP, JPP
     J2 = JP
     IF ((M.GE.I7STRT(JP)).AND.(M.LE.IZSTOP(JP))) GO TO 1320
1310 K1 = K1 + 1
     IF (NSSW2.EQ.0) 30 TO 3010
     WRITE(6, FMT) DIST(J), COUNTS(J), RACK?(J)
     GG TO 3010
1320 00 1330 JP = J2, JPP
     IF ((M.LT.IZSTRT(JP)).OR.(M.GT.I7STOP(JP))) GO TO 1340
     JB = JQB + JP
     PKRACK(JR) = PKRACK(JR) + RACK2(J)
1325 K2 = K2 + 1
     ITT = M - I7STRT(JP) + 1
     STORV1(J) = STORV1(J) + STORZ(IT[,J^2])
     STORZ(ITT, JP) = STORZ(ITT, JP) + BACK2(J)
1370 S(K2) = STORZ (ITT, J2)
1340 \text{ FMT}(3) = WORD(K1 + 1)
     IF (NSSW2.E0.0) 30 TO 3010
3019 WRITE(6,FMT) (DIST(J),COUNTS(J),S4CK2(J),STORV1(J),(S(K),K=1,K2))
3010 CONTINUE
     MTT = MMX + 1
3300 CONTINUE
     JOB = JOB + NT
  32 IF (NSSW2.E0.0) 30 TO 3401
     DO3400 I=MTT, NCHANN
3400 WRITE(6, FMT) DIST(I), COUNTS(I), 343(2(I)
        ... PRINT FEADINGS ...
3401 WRITE(6,85) (TITLE(I), J=1,8 ), TODAY
     WRITF(6,200)
 550 DO 560 I=1,JC
     IPF = IBLNK
     IF (IFIXPK(I).GT.0) IPF = ISF
     AREA = XSECTS(I) +PK34CK(I)
     STXEPR = 0.
     IF (AREA.GT.O.) STXERR = SORT(AREA)
     WRITE(6, 212) PEKPOS(I), IPF, PEKERR(I), XSECTS(I), XSECER(I),
    1 PKEACK(I), STXERR
 550 CONTINUE
     DEVST=DEVSO= C. 0
```

```
AUNK=ARES=0.0
     DO 5000 IJK=1, MAXREF
     AUNK = AUNK + COUNTS (IJK)
     ARES = ARES+STORV1 (IJK)
     DEVSO=DEVSQ+(COUNTS(IJK)-STORV1(IJK)) **2
5030 CONTINUE
     DEVST=SORT (DEVST)
     PRINT+," AREA UNKNOWN = ", AUNK," AREA RESOLVED = ", ARES," RMS ERR
    COR = ", DEVST
     RETURN
  55 FORMAT(1H1,1X,8A10,10X,A10)
 200 FORMAT (/6X4HPEAK, 23X3H ,19X5HNJ43., 35X4HEST./4X8HPOSITION, 5X7H
                      ,5X5HERROR,7X6HCJUNTS,12X5HERROR,13X1GHRACKGROUND
    1
           ,6X6H
    2,6X5HERROR/)
 201 FORMAT(3XF9.3,1X41,3XF8.4,4XF8.4,4XF5.2,5XF9.2,3(4XF9.2))
 202 FORMAT (F9.+, 1X, 2=10.4, 2F10.2, F3.2, =3.1, 3X45, F5.1)
 221 FORMAT(3XF9.3,1X41,3XF8.4,16XF6.2,5XF9.2,3(4XF9.2))
 222 FORMAT (F9.4, 1XF10.4, 10X, 2F10.2, F3.2, F8.1, 3XA6, F5.1)
 212 FORMAT (3XF3. 3,1X41,26XF6.2,5XF12.2,3(4XF11.2))
 215 FORMAT (F9.+, 21X, 271). 2, F8.2, F8.1, 3X46, F5.1)
 230 FORMAT (2H-1)
     END
```

```
SUBROUTINE SPCTRM
 ... READS THE SPECTRUM CARDS AND SETS THE DISTANCE AND COUNT ARRAYS
    DIMENSION YSAV(10)
    COMMON/DATA/X(2100), Y(2100), RUNID, TODAY, FRED, DELX, NOFTEN,
   1 N, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
    COMMON JOPIN/ KEPREF, KEPDAT
..... INITIALIZE COUNTS ARRAY TO ZERO
    DO 100 I=1,2100
100 Y(I)=0.0
    N=10
    DELX = 1.0
    PRINT*," ENTERED SPECTRUM, CALLING ROSPEC"
    CALL RDSPEC (Y, N, NT AG, MAXREF)
    IF(N.GT.2100) GO TO 235
    D1=0.0
    GO TO 250
275 WRITE (6,2) N
2:5 IERR=1
    GO TO 300
        SET THE DISTANCE VALUES
....
250 X(1)=01
    00 260 I=2, N
25 0 X(I) = D1 + FLOAT(I-1) * DELX
300 RETURN
30 FORMAT (F6.0, 9F7.0, 8XF3.0)
    FORMAT (6HO D = , = 3.7, 16H LESS THAN 31 = , = 9.3)
    FORMAT (1140 NCHANN = , I5, 18H GREATER THAN 2100)
5
    FORMAT (F5.0/10 (FE.0,2X))
```

```
SUBROUTINE REFPEK
C
      DETERMINES THE PARAMETERS OF THE REFERENCE PEAK
      COMMON /402/ DUMANS(161), STORV1(2130), RAWX(2100), ITIMES, NNX
      COMMON /403/ SKIP(55),LO
      COMMON /40+/ INTREF(20,10),STORFF(2100),DELTA1,DELTA2,DELTA3,
        STOIPR, REFMAX, IN1, ID2, IDT, N3, NE, NREF
      COMMON /A05/ BACY2 (2100), DR (50), 34CK (50), NJ, NBACK, NPKRO
      COMMON /DATA / DIST(2100), COUNTS(2100), RUNID, TODAY, FRED, OFTEN,
       NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IFRR, MAXREF, MAXP2
      COMMON JOPINI KEFREF, KEPDAT
      IF (LQ) 10, 30,10
   10 IF (NREF) 300,201,300
   30 IF (NREF) 100,201,80
   SELECT REFSHAPE FROM INTERNAL DATA
  90 no90 I=1.20
   30 STOREF(I) = INTREF(I, NREF)
   FIND LOWER EDGE OF PEAK
  100 D0110 I=1. MAXREF
      IF(STOREF(I)) 110,110,120
  110 CONTINUE
  120 IMIN = I
      IF (I.GT.1) IMIN = I - 1
    FIND UPPER EDGE OF PEAK
      I = MAXREF
  130 IF (STOREF(I)) 1+0,140,150
  140 I=I-1
      GO TC 130
  170 IMAX = I
      IF(I.LT.MAXREF) IMAX = I+1
    FIND TOP OF PEAK
      REFMAX=0.0
      DO 170 I=IMIN, IMAX
      IF (REFMAX-STORE=(I)) 160,170,17)
  150 REFMAX = STOREF(I)
      ITOP=I
  1' 0 CONTINUE
      SREF = .001* REFMAX
    FINDS THIRD HEIGHT
      REFTHD = REFMAX/3.
      DO 180 I=ITOP, IMAX
      IF (STOREF(I)-REFTHD) 190,180,180
  13 0 CONTINUE
  190 RI=I
      OFFSET = (REFTHO-STOREF(I))/(STOREF(I-1)-STOREF(I))
      RTHPOS=RI-OFFSET
      DELTA1 = (FLOAT(JMAX)-RTHPOS) + OFFEN
      DELTA2 = (RTHPOS-FLOAT (IMIN))+OFTEV
      DELTA3 = (RTHPOS-FLOAT (ITOP)) +OFFEN
      RTHPOS = (RTHPOS-1.0) *OFTEN
      STORE = 0.0
  210 IDT = (DELTA2+DELTA1) / OFTEN + 1.1
      ID1= (DELTA1 + DELTA3) /OFTEN +0.1
      ID2=(DELTA2-DELTA3)/OFTEN +.1
      NE = NCHANN - ID1
      N9 = ID2 + 1
      IF (NREF) 230,210,230
    SELECT REFSHAPE FROM RAW SPECTRUM
```

```
210 KU = (STOIPR-DIST(1))/OFTEN + 0.1
    IID = KU - ID2
    IMIN = 1
    IMAX = IMIN + IDT - 1
    STORE = UFTEN*FLOAT(IIn) + DIST(1)
    RTHPOS = STOIPR + DELTA3
    DO 220 IR=1, IDT
220 STOREF(IR) = RAWX(IID+IR)
230 IF (LQ) 240,240,300
2' 0 00 250 I=IMIN, IMLX
250 STOREF(I-IMIN+1) = STOPEF(I)
    DO 255 IM=ITOP, IMAX
275 IF(STOREF(IM).LT.SREF)STOREF(IM)=0.0
    IM=IMAX-1MIN+2
    DO 2EO I=IM, MAXREF
250 STOREF(I) =0. C
    IF (NNX) 400,400,300
300 WRITE(6, 310) DELTA1, DELTA2, DELTA3
310 FORMAT (11H0 DELT&1 = ,F9.2,8X9HDELTA2 = ,F9.2,8X9HDELTA3 = ,F9.2)
PRINT*," IDT = ",IDT," ID1 = ",ID1." ID2 = ",ID2
    WRITE(6,350) RTHPOS
350 FORMAT (32H REFERENCE PEAK THIRD HEIGHT = , F9.4)
400 RETURN
    END
```

FUNCTION PPOISS(NORS, AVERAG)

1 PPOISS=((AVERAG*'NORS)/FACTOR(NORS))*EXP(-AVERAG)
RETURN
END

SUBPOUTINE OUTPUT(X,NMAX)
DIMENSION X(1)
IMAX=NMAX/10
DO 100 K=1,IMAX
I1=K'10
I0=I1-9
100 PRINT 200,(X(I),I=I0,I1)
200 FORMAT(5X,10(E9.3,2X))
RETURN
END

```
SUBROUTINE BIRND
      ... CALCULATES THE BACKGROUNDS ...
C
      COMMON /A02/ DE(32), RHO2(52), M(50), X(10), A(10,10), DUMMY(4099)
      COMMON /403/ TIT_E(20), PEAK(20), 3_N((23), NPFAK, NCALC, IGS, LQ
      COMMON /A04/ INTREF(20,10), STOREF(2100), DELTA1, DELTA2, DELTA3,
     1 STOIPR, REFMAX, ID1, ID2, IDT, N3, NE, NREF
      COMMON /A05/ RAC(2(2100), DB(50), BACK(FO), NJ, NBACK, NPKRD
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FRED, OFTEN,
     1 NOFTEN, NCHANN, SKIP (5), MAXREF, MAXP2
      qq = DIST(1)
      IF (NBACK-1) 10,700,900
         ... AUTOMATIC BACKGROUND SELECTION ...
   10 NP = NPEAK + 1
      IJ = 0
      NJ = 1
      RH02(NJ) = 1.E10
      DO 200 JJ=1, NP
      IJ = IJ + 1
      IF(IJ-NP) 20,30,:00
   20 LOCPK = (PEAK(IJ) - DELTA3-QO) /OFTEN + 1.1
      IF(IJ-1) 40,40,60
   +0 NDEL = LOCPK - ID2 - 1
      MA = 0
      GO TO 100
   50 NOEL = IFIX((PEA<(IJ)-PEAK(IJ-1))/)=TEN + 0.1) - IOT
      MA = LCCPK - ID2 - NOFL - 1
      GO TO 100
   30 LOCPK = (PEAK(IJ-1)-DELTA3-00)/OFFEN + 1.1
      NDEL = NCHA IN - _DCPK - ID1
      MA = LOCPK + ID1
  100 IF (NOEL-10) 200,120,120
  120 JBACK = FLOAT (NDEL)/10.0 + 0.2
      JP = NDEL/JBACK
      SHIFT = FLOAT (JP)/2.
      DO 160 I=1, JRACK
      NJ = NJ + 1
      9 = 0.0
      DO 140 IP=1, JP
  140 B = P + COUNTS (M4+IP)
      RHO2(NJ) = 9/FLO4T(JP)
      BACK(NJ) = RHO2(NJ)
      CHECK = RHO2(NJ-1) + 2. *SORT(RHO2(NJ-1)+1.)
      IF (RHO2(NJ)-CHECK) 160, 160, 150
  150 NJ = NJ - 1
      GO TO 170
  150 DE(NJ) = DIST(MA+1) + OFTEN+SHIFT
      DB(NJ) = DE(NJ)
          ... TEST FOR LIMIT OF 50 POINTS AND TAKE APPROPRIATE ACTION ...
  170 IF (NJ-49) 180,175,+00
  175 IF (IJ.GE.NP) GO TO 400
      IJ = NP
      GO TO 80
  130 MA = MA + JP
  200 CONTINUE
  400 IF (NJ-5) +10,420,420
  +10 M = NJ - 1
```

GO TO 430

```
420 M = L
  430 N = NJ
  500 MM = M + 1
      DO 510 I=1, N
  510 W(I) = 1.0
      CALL LSQPOL (N, MM)
      DO 54 G I=1, NCHANN
      BACK2(I) = X(1)
      DO 520 IP=1,4
  520 BACK2(I) = BACK2(I) + X(IP+1)+DT3T(I) ++IP
      IF(BACK2(I)) 530,540,540
  530 BACK2(I) = 0.0
  5+0 CONTINUE
      GO TO 800
          ... INTERPOLATE THE PACKGROUND THROUGH THE POINTS READ IN ...
C
  700 JC1=0
      JC2=0
      IF(DB(1)-DIST(1)) 710,710,705
  705 JC1=1
      DE(1) = DIST(1)
      RH02(1)=BACK(1)
  710 IF(DB(NJ)-DIST(NCHANN)) 715,750,750
  715 JC2=1
      DE(NJ+JC1+1) = DIST(NCHANN)
      RHO2 (NJ+JC1+1) = 840K(NJ)
  750 DO 755 I=1, NJ
      DE(I+JC1) = DB(I)
  755 RH02(I+JC1) = BACK(I)
      N=NJ+JC1+JC2
      IF (N.LT.3) GO TO 900
      J=2
      DO 790 I=1, NCHANN
      DIX = DIST(I)
  770 IF(DIX-DE(J+1)) 750,775,775
  775 J=J+1
      IF (J.GE.N) J= J - 1
  780 DEM1=(DE(J-1)-DE(J)) * (DE(J-1)-DE(J+1))
      DEM2= (DE(J) - CE(J-1)) * (DE(J) - DE(J+1))
      DEM3=(DE(J+1)-DE(J-1))* (DE(J+1)-DE(J))
      BACK2(1)=(DIX-DE(J))*(DIX-DE(J+1))/DEM1*R+02(J-1)
          + (DIX-DE(J-1)) * (DIX-DE(J+1)) / JE42*RHJ2(J)
     1
          + (DIX-DE (J-1)) * (DIX-DE(J)) /DE43* RH02 (J+1)
      IF (BACK2(I).LT.0.0) 3ACK2(I)=0.0
  720 CONTINUE
  800 WRITE(6,310) (OF(I), RHO2(I), I=1. VI
  $10 FORMAT (26HOPOINTS USED BY BACKGROUND/ (2F12.3))
      GO TO 1000
          ... CALCULATE THE BACKGROUND INTERVALS...
C
  900 IJ = 2
      09(1) = DIST(1)
      IF (NJ.EQ.1) DB(2) = DIST(NCHANN) + DFTEN
      DO 920 I= 1, N CHANN
      IF (DIST(I).GE.DB(IJ)) IJ = IJ + 1
      IF (IJ.EQ.NJ) D9(VJ+1) = DIST(NC+1VV) + DFIEN
  320 BACK2(I) = BACK(IJ-1)
      WRITE(6,930)
                      DISTANCE, 17X11H BACKGROUND)
  930 FORMAT (13H)
```

```
END
      SUBROUTINE L SQPOL (NSUB, MSUB)
      LEAST SQUARE POLYNOMIAL FIT
C
      COMMON /A02/ X(52), Y(52), W(50), B(10), A(10,10), XPOWER(50),
     1
       DUMMY (4049)
      N=NSUB
      M=MSUR
      M1=H+1
      M3=M+M+M
      M31=M3-1
      M41=M31+4
C
      FORMATION AND INVERSION OF SYSTEM OF NORMAL EQUATIONS
C
      00 100 K2=M1,M41
      XPOWER (K2) = 0.0
  100 CONTINUE
      DC 200 K1=1,N
      TERM=W(K1)
      DO 200 K2=M1,M31
      XPOWER (K2) = T ERM+XPOWER (K2)
      TERM=X(K1) + TERM
  200 CONTINUE
      00 300 I=1, M
      00 300 J=1, M
      K2=I+J+M-1
      A(I, J) = XPOWE F(K2)
  300 CONTINUE
      DO 400 K=1, N
      TERM=W(K) +Y(K)
      DO 400 K2=M3,M41
      XPOWER (K2) = T ERM+XPOWER (K2)
```

00 94 0 I=1, NJ

TERM=X(K) +TERM

B(I) = XPOWER(K2)

CALL MATINY (A, M, 3, 1, DETERM, 10)

DO 500 I=1, M K2=I+M31

400 CONTINUE

FOO CONTINUE

730 CONTINUE RETURN

END

. ()

1000 RETURN

DIX = DP(I+1) - OFTEN

940 WRITE(6,950) (DB(I),DIX,BACK(I)) 950 FORMAT(F9.3,14-,F8.3,14XF6.2)

```
SUBROUTINE PREFAR
      ...CONVERTS CATA TO CHANNEL NUMBERS AND PREPARES IT FOR THE
        VAPIABLE-METRIC PACKAGE ...
      REAL LPF
      COMMON /400/ HH(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
        GB(20), F9, GS, E_, SL, FP, GSP, T0, Z7Z, D, AA, 3SS, F0, GTP, FB, GTT, GSR,
        DELTA, EE, LT, MS, IT, L, THOLD (20), NSSW1, NSSW2
      COMMON/A01/7 (2102, 10), 98 (2102), T75TRT (20), TZSTRP (20), R(2102),
        X(2100), W(2100), E(2100), C(20,20), A(20), G(20), ERR(20), DEL,
        REP, F, FBFST, LPF(22), LP(22), IRS, IPR, IPRE, IIC, ITC, IOFF
      COMMON /402/ SIGM4 (20), ERRZ (20), PERSTO (21), STORHH(20),
        XINTIS(20), INDEX(20), INITAL(20), IFINAL(20), STORV1(2100),
        RAWX (2100) , ITIMES, MNX
      COMMON /A03/ DUMMY (53) , NT , NCALC , ISS, LQ
      COMMON /A04/ INTREF(20,10), STOREF(2100), DELTA1, DELTA2, DELTA3,
       STOIPR, REFMAX, ID1, ID2, IDT, N3, NE, NREF
      COMMON /JATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, DETEN,
       SKIP(7), MAXREF, MAXP2
      DEL = 0.1
      QQ = DIST(1)
C
         ... CONVERT ALL UNITS TO CHANNEL NUMBER...
      DO 1060 I=1, NT
      PERSTO(I) = (PERSTO(I) -00) /OFTEN + 1.0
 1050 STORHH(I) = 1.0
      PERSTO (NT+1)=3000.0
      DEL3 =AINT (DELTA1+DELTA2+0.1)
      IPR= (2.0+DELTA2)
      IPRE=((2.0+DELT42) -=LOAT(IPR))*10.0
      DO 1061 I = 1, MAX 2
 1051 R(I)=0.0
      DO 1065 I=1, IDT
 1035 R(I+1) = STOREF(I)
      IRS = IDT + 1
      I1C=1
      ITIMES=0
      III = 1
         III = (NUMPER OF PEAKS ALREADY AVALYZED) + 1
 2000 IOFF = III - 1
         ... DIVIDE GROUP OF PEAKS INTO NON-OVERLAPPING SURGROUPS ...
      MS=0
      IF (III-NT) 20 01, 2001, 3000
         I1CSS = (FIRST CHANNEL NUMBER OF FIRST PEAK IN SUBGROUP) - 1
 2001 IICSS = PERSTO(III) - DELTA2 + 0.1
      IF(I1CSS.GT.1) I1CSS = I1CSS - 1
      DO 2015 JJ=1,20
      LT=LT+1
      IF (PERSTO
                  (III+JJ)-PERSTO (III+JJ-1)- DEL3) 2015,2015,2020
 2015 CONTINUE
2020 XXX = PERSTO(III)
         ITC = TOTAL NUMBER OF CHANNELS IN THE SUBGROUP
      ITC = PERSTO(LT+JOFF) - XXX + DE_T41 + DELTA2 + 3.1
         ... SETUP INITIAL MATRIX, DATA, WEIGHTS, AND PARAMETERS...
      DO 2025 I=1,LT
      DO 2025 J=1, LT
 2025 HH(I,J)=0.0
      DELTA=1.0
```

```
DO 2030 I=1.LT
      IM = IOFF + I
      PER(J) = PERSTO(IM) - XXX + DELTA2 + 2.
      HH(I, I) = STOR + H (! 4) ** 2
      IF (IHOLD(IM)) 2028,2028,2027
 2027 HH(I,I) = 0.0
      GO TC 2030
 2028 DELTA = DELTA HH(I,I)
 2070 CONTINUE
      DO 2035 I=I1C,ITC
      JJ = I + I1CSS - 1
      X(I) = RAWX(JJ)
2035 W(I)=1.0/SQRT(X(I)+10.0)
      EE = FLOAT(ITC-LT) *0.05
      CALL DAVIDY
      ITIMES=ITIMES+1
         INDEX = NUMBER OF PEAKS IN SUBGROUP
C
         INITAL = STARTING CHANNEL NUMBER IN SUBGROUP
C
         IFINAL = FINAL CHANNEL NUMBER FOR SURGROUP
C
      INDEX (ITIMES) = LT
      INITAL (ITIMES) = 11088
      IFINAL (ITIMES) = [1088 + ITC - 1
      03 = ITC - LT
      ...CALC. ERRORS IN POSITIONS AND COMPUTE NORMALIZED INDIV. PEAKS
C
      DO 2042 I=1, LT
      IM = IOFF + I
      PERSTO (IM) = (PER(I) +XXX-DELTA2-3.01 * OFTEN + QO
      STORHH(IM) = HH(I, I)
      SIGMA(IM)=SQRT (48S ((2.0*STORHH (IH)*FREST)/Q3))*OFTEN
      IF (A(I)) 2115, 2110, 2115
 2110 ERRZ (IM) = 0.0
      GO TO 2120
 2115 ERRZ (IM) = ERR (I) /4 (I)
 2170 DO 2040 J=1, MAXP2
 2040 \ Z(J,IM) = Z(J,IM)*A(I)
 20 2 CONTINUE
      IF (IT.GE.25) WRITE(6,1001) (PERSTO(I),I=1,LT)
      III = III + LT
      GO TO 2000
 3010 RETURN
 1001 FORMAT(51HD EPSILON TOD SMALL - CANNOT CONVERGE FOR PEAKS AT ,5F10
     1.2/(10F10.2))
      END
```

```
SUBROUTINE FCN(LLTT, 3F, F9, PER, M1)
C
      ... SETS UP THE LINEAR EQUATIONS AND DRIVEN RELATIVE PEAK HEIGHTS.
      REAL LPF
      DIMENSION PER (20), 63 (20)
      COMMON/A01/7(2102, 1)) ,SS(2102) ,I75TRT (20) ,IZSTOP (20) ,R(2102) ,
       X(2100), W(2100), E(2100), C(20,20), A(20), G(20), ERR(20), DEL,
     2 REF, F, FBEST, LPF(22), LP(22), IRS, IPR, IPRE, I1C, ITC, IOFF
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FRED, OFTEN,
     1 NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
      LT=LLTT
      IF (M1.EQ.1) FBEST = 1.0510
 4006 DO 91 L=1,LT
      LP(L) = FER(L)
      LPF(L) = (PER(L) -FLOAT(LP(L)))*10.0
   91 CALL SHIFT(L)
      PRINT+," IF M1 = 3 = ",M1," WILL CALL FUN FROM FON "
  205 IF (M1-3) 222,213,222
         DUMMY CALL TO FUN TO FORM THE ARRAY E
  219 CALL FUN(LT)
      DO 220 I=I1C,ITC
  220 W(I) = 1.0/SGRT(A3S(E(I))+10.)
  222 DO 210 M=1.LT
      MM = M + IOFF
      DO 210 L =1, M
      LL = L + IOFF
      C(M,L) = 0.0
      DO 200 I=I1C,ITC
      IF ((I.LT.IZSTRT(LL)).OR.(I.GT.IZSTDP(LL))) GO TO 200
      IF ((I.LT.IZSTRT(4M)) .OR.(I.GT.IZST)?(MM))) GO TO 200
      IL = I - I7STRT(LL) + 1
      IM = I - IZSTRT(MM) + 1
      C(M,L) = C(M,L) + W(I)*W(I)*Z(IL,LL)*Z(IM,MM)
  200 CONTINUE
  210 C(L,M) = C(M,L)
      DO 201 M=1, LT
      MM = M + IOFF
      A(M) = 0.0
      DO 201 I=I1C.ITC
      IF ((I.LT.I 75TRT(MM)).OR.(I.GT.I75T)P(MM))) GO TO 201
      IM = I - I7STRT(44) + 1
      A(M) = A(M) + W(I) + W(I) + X(I) + Z(IM, MM)
  201 CONTINUE
      CALL MATINV(C, LT, 4,1, DETERM, 5)
      CALL DERIVP(LT, PER)
      DO 1600 L=1,LT
 1600 GR(L) = G(L)
      PRINT+," CALLING FUN FPOM FCN, " = ",F," GR=G= ",G
      CALL FUN(LT)
      IF(M1-3) 206,1011,206
 1011 F7 = F/(ITC-I1C-_{\Gamma})
      DO 1006 L=1,LT
      REP = F7+C(L,L)
1006 ERR(L) = SORT(ASS(REP))
  206 F9 = F
      IF (F9.LT.FBEST) FREST = F9
      RETUPN
```

```
SUBROUTINE DERIVP(LLTT, PER)
   ... CALCULATES DERIVATIVES OF FUNCTION F(FUN) WITH CHANGE
   IN POSITION
   REAL LPF, LOPE
   DIMENSION PER(20)
   COHMON/A01/7 (2102, 10), SS (2102), IZSTRT (20), IZSTOP (20), R(2102),
  1 X(2100), W(2100), E(2100), C(20,20), A(20), G(20), ERR(20), DEL,
  2 REP, F, FBEST, _PF(22), LP(22), IRS, IPR, IPRE, I1C, ITC, IDFF
   COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
  1 NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
   LT=LLTT
   DO 9 EL = 1, LT
   LL = L + IOFF
   DO 94 I=1, MA XP2
34 SS(I) = Z(I, LL)
   ISAV1 = IZSTRT(L_)
   ISAV2 = IZSTOP(L_)
   LOP=LP(L)
   LOPE=LPF(L)
   Y=PEF(L)+DEL
   LP(21) = Y
   LPF(21) = (Y-FLOAT(LP(21)))*10.0
   Y=PER(L)-DEL
   LP(22) = Y
   LPF(22) = (Y-FLOAT(LP(22)))*10.0
   LP(L)=LP(21)
   LPF(L) = LPF(21)
   CALL SHIFT(L)
   PRINT+," CALLING FUN FROM DERIVP, L = ",L," F = ",F
   CALL FUN(LT)
   FP=F
   LP(L)=LP(22)
   LPF(L)=LPF(22)
   CALL SHIFT (L)
   PRINT*," CALLING FUN FROM DERIVP, FD = F = ",F
   CALL FUN(LT)
   G(L) = (FP-F) /(2.0'DEL)
   DO 95 I=1, MAXP2
95 Z(I,LL) = SS(I)
   IZSTFT(LL) = ISAV1
   IZSTOP(LL) = ISAV2
   LP(L)=LOP
36 LPF(L)=LOPE
   RETURN
   END
```

C

```
SUBFOUTINE SHIFT (.0)
      ... CONTROLS INTERPOLATION OF FRF. PEAK FOR SHIFTING FRACTIONS
C
C
      OF CHANNELS
      ... CENTROLS INTERPOLATION OF REF. PEAK FOR SHIFTING FRACTIONS OF C
      REAL LPF
      COMMON/A01/7 (2102, 10), SS (2102), IZSTRT (20), IZSTOP (20), R (2102),
     1 X(2100), W(2100), E(2100), C(20,20), A(20), G(20), ERF(20), DEL,
     2 REP, F, FREST, _PF(22), LP(22), IRS, IPR, IPRE, I1C, ITC, IOFF
      COMMON /DATA / DIST(2100), COUNTS(2100), RUNID, TODAY, FRED, OFTEN,
     1 NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
      L=LD
      LL = L + IOFF
      C1=LF(L)
      C2=LPF(L)
      U=C1+C2/10.0
      B8=IFR
      P9=IFRE
      DO 100 J=1, MAX F2
  100 Z(J,LL) = J.0
      P1=B8+P9/10.0
      IF (81-U) 300,18,3
C
      SUBROUTINE SHIFTL L LESS THAN R
    9 J=1
      IZSTRT(LL) = 1
      IF (IPRE-LPF(L)) 10,11,12
   10 F = 10 + IPRE - LPF(L)
      I = IPR-LP(L)
      GO TO 14
   11 F=0.0
      GO TO 13
   12 F = IPRE-LPF(L)
   13 I = IPR-LP(L)+1
   14 F1 = F/10.0
   15 Z(J_*LL) = R(I) + F1*(R(I+1)-R(I))
      I=I+1
      J=J+1
      IF (I-IRS) 15,15,17
   16 IF (J-ITC) 15,15,17
   17 IZSTOP(LL) = J - 1
      GO TO 23
      SUBROUTINE STIFTO L EQUAL R
C
   18 DO 20 J=1, IRS
   20 \ Z(J,LL) = R(J)
      IZSTRT(LL) = 1
      IZSTOP(LL) = IRS
      GO TO 23
      SUBROUTINE SHIFTR R LESS THAN L
  300 I=1
      IF (IPRE-LPF(L)) 1,2,3
    1 F = 10 + IPRE - LPF(L)
      K = LP(L)-IPR+2
      GO TO 5
    2 F=0.0
      GO TO 4
    3 F = IPRE-LPF(L)
    4 K =LP(L)-IPR+1
    5 F1 = F/10.0
```

```
IZSTRT(LL) = K
      J = 1
    6 \ Z(J,LL) = R(I) + F1*(R(I+1)-R(I))
      I=I+1
      J=J+1
      K = K + 1
      IF (I-IRS) 7,7,3
    7 IF (K-ITC) 5,6,8
    8 IZSTOP(LL) = K - 1
   23 RETURN
      END
       SUBROUTINE FUN(LT)
       ... CALCULATES THE FUNCTION F WHICH IS BEING MINIMIZED...
C
       REAL LPF
      COMMON/A01/Z (2102, 10), SS (2102), I73TRT (20), I7STOP (20), R(2102),
      1 X(2100), H(2100), E(2100), S(20,20), A(20), G(20), ERR(20), DEL,
     2 REP, F, FBEST, LPF(22), LP(22), IRS, IPR, IPRE, 110, ITC, IDFF
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
     1 NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR, MAXREF, MAXP2
       F=0.0
       DO 60 I=1, ITC
   50 E(I) = 0.0
       DO 70 L=1,LT
       I1 = IZSTRT(L+IOFF)
       I2 = I7STOP (L+IOFF)
       0 I=I1, I2
       J = I - I1 + 1
   70 E(I) = E(I) + A(_) + 7(J, L + IOFF)
       DO 80 I=I1C, ITC
       F1 = (X(I) - E(I)) \cdot W(I)
   30 F = F + F1*F1
       RETURN
       END
      SUBROUTINE ARYODR (A, B, N, L)
         OPDERS THE ARRAY 4, AND MAKES SAME OF DERING TO B IF L=2.
C
      INTEGER B
      DIMENSION 4(1),9(1)
      NP = N - 1
      DO 50 I=1, NP
      K = I + 1
      DO 50 J = K, N
      IF (A(I)-A(J)) 50,50,20
   20 IF (L-1) +0,40,30
   30 \text{ ISAV} = B(I)
      B(I) = B(J)
      B(J) = ISAV
   40 SAVE = A(I)
      A(I) = A(J)
      A(J) = SAVE
   FO CONTINUE
      RETURN
      END
```

```
SUBROUTINE MATINV(4, NSUB, B, MSUB, JET, NMAX)
C
       DIMENSION A (NMAX, NSUB), B (NMAX, MSJB)
       DIMENSION PIVOT(100), INDEX(100), [PIVOT(100)
       EQUIVALENCE (PIVOT, INDEX, IPI VOT), (AMAX, T), (IROM, 11, IRC),
                     (TEMP, SHAP)
     1
       DATA (ISHIFT=4095), (MASK=0000000777777778)
C
       N=NSUB
       M=MSUB
C
C
       INITIALIZATION
C
      DETERM=1.0
       00 20 I=1.V
       IPIVOT(I)=0
   20 CONTINUE
       DO 550 I=1, V
C
C
       SEARCH FOR PIVOT ELEMENT
C
       AMAX=0.
       DO 105 J=1.N
       TEMP=IPIVOT (J) . AND . . NOT . MASK
       IF (TEMP) 105,60.
   EO DO 100 K=1, N
       TEMP=IPIVOT (K) .AND .. NOT . MASK
       IF (TEMP) 100,80
   30 TEMP=ABS (4 (J,K))
       IF (TEMP-AMAX) 100,85,85
   35 IROW=J
       ICOLUM=K
       AMAX=TEMP
  100 CONTINUE
  105 CONTINUE
       INDEX(I) = IND EX(I) + (ISHIFT*IROW+ICOLJM)
       J=IROW
       AMAX=A (J, ICOLUM)
       DETERM=AMAX * CETERM
C
C
       MATRIX SINGULAR
C
       IF (DETERM) 110,500
C
  110 PIVOT (ICOLUM) = INDEX (ICOLUM) . OR . A MAX. AND . . NOT . MASK
C
C
       INTERCHANGE ROWS
C
       IF (IFOW-ICOLJM) 1+0,260
  140 DETERM =- DETERM
       DO 200 K=1, N
       SWAP = A (J, K)
       A(J,K)=A(IGOLUM,K)
       A (ICCLUM, K) =SWAP
  200 CONTINUE
       DO 250 K=1, M
       SWAP=B(J,K)
```

```
B(J,K)=B(ICOLUM, <)
       B(ICOLUM, K) = SWAP
  25 0 CONTINUE
CC
       DIVIDE PIVOT ROW
C
  250 K=ICCLUM
       A(ICOLUM, K) = 1.0
       DO 35 0 K=1, N
       A (ICCLUM, K) = A (ICOLUM, K) / AMAX
  35 0 CONTINUE
       DO 370 K=1, M
       B(ICCLUM, K) = B(ICCLUM, K) / AMAX
  3"0 CONTINUE
C
C
       REDUCE
C
       DO 550 J=1, N
       IF (J-ICOLUM) 400,550
  400 T=A(J, ICOLUM)
       A(J, ICOLUM) = 0.0
       00 45 0 K=1, N
       A(J,K)=A(J,K)-A(ICOLUM,K)+T
  450 CONTINUE
       DO 500 K=1, M
       B(J,K)=B(J,K)-3(ICOLUM,K)*T
  500 CONTINUE
   550 CONTINUE
C
       INTERCHANGE
C
C
  500 DO 710 I=1, N
       I1=N+1-I
       IRC=INDEX(I1).AND.MASK
       K=IRC/ISHIFT
       ICOLUM=IRO-K*ISHIFT
       IF(K-ICOLUM) 650,710
   6=0 DO 705 J=1, N
       SWAP=A(J,K)
       A(J,K) = A(J,ICOLUM)
       A(J, ICOLUM) = SWAP
   705 CONTINUE
   710 CONTINUE
   740 DET=DETERM
C
       RETURN
       ENTRY OMATINV
       RETUFN
       END
```

```
SUBROUTINE DAVIDY
    ...THIS IS THE CONTROL ROUTINE FOR THE VARIABLE-METRIC PACKAGE...
    COMMON /A00/ H(2[,20), Y(20), G(20), S(20), X^{2}(20), GP(20), T(20),
   1 GB(20), F, GS, EL, SL, FP, GSP, TA, Z, 7, 4, 3SS, FO, GTP, FB, GTT, 3SB,
   2 DELTA, E, N, MS, II, L, IHOLD (20), NSSW1, NSSW2
 15 M1=1
    IT = 0
    F=0.0
    CALL FCN(N,G,F,X,M1)
    IF (NSSW1) 20, 25,20
 20 WRITE(6,3) IT, MS, F
    GO TO 840
120 M1=2
200 CALL READY
                                     L= ",L
    PRINT+,"
                 CALLED READY
    GO TO (800,300,500,500), L
300 CALL AIM
    PRINT+,"
                  CALLED AIM
                                     L= ",L
    GO TO (400,500,500,300), L
400 CALL FIRE
    GO TO (500,500,300,300), L
500 CALL DRESS
    IF (IT-25) 120,550,550
550 M1 = 3
    GO TO 900
900 M1=3
    IF (NSSW1) 22, 25, 22
 22 WRITE (6, 11)
810 DO 820 II=1, N
320 WRITF(6,7) (H(II, JJ), JJ=1,N)
830 WRITE (6, 12) CELT4, F, GS
840 IF (NSSW1) 24,25,24
 24 WRITE(6,10) (X(I), I=1,N)
    GO TO (850,850,850), M1
850 WRITE(6, 13) (G(I), I=1, N)
950 WRITE(6,9)
 25 GO TO (120,120,900), M1
900 IF (N.GT.1) CALL DRIER
    CALL FCN(N,G,F,X, 41)
 30 RETURN
  3 FORMAT (6E12.5)
  7 FORMAT (1H08E14.5)
  8 FORMAT (4HOIT 14,7H STEP 14,4H == E14.5)
  9 FORMAT (20H0 - - - - - - - - -)
 10 FORMAT(3H0X=3E14.5/(3H0 8E14.5))
 11 FORMAT (1340 FINAL VALUES/1340 ERROR MATRIX)
 12 FORMAT (740) ELTA=E14.5, H F=E14.5, 54 GS=E14.5)
 13 FORMAT (3HOG=bE14.5/(3HO BE14.5))
```

SUBROUTINE READY COMMON /400 / H(20, 20), Y(20), G(20), S(20), $X^{2}(20)$, GP(20), T(20), G8(20), F, GS, EL, SL, FP, GSP, T0, Z, 7, A, GSS, F0, GTP, F8, GTT, GSB, DELTA, E, N, MS, II, L, IHOLD (20), NSSA1, NSSW2 200 L=1 CALL MATMPY (N,N,H,G,S) DO 205 I=1, N 205 S(1) =-S(1) CALL MATMPY (1,N,S,G,GS) IF (65+E) 210,240,240 210 L=2 EL=2.0 TO=EL +F/GS IF (TO+EL) 213, 213, 212 212 EL =- TO 213 SL=-GS DO 215 I=1, N 215 XP(I)=X(I)+EL+S(I) CALL FCN(N, GP, FP, XP, 2) CALL MATMPY (1, N, S, G2, GSP) IF (-GSP) 240,240,220 220 IF (F-FP) 240,240,225 225 L=3 IF (NSSW1) 100,101,100 100 WRITE(6,1) 101 F9=FF DO 230 I=1,N GB(I) = GP(I) T(I) = XP(I)230 CONTINUE IF (EL-2.0) 240,235,240 235 L=4 DELTA = DELTA + CELTA T0=1.0/SL 240 RETURN 1 FORMAT (10HOUNDERSHOT) END

SUBROUTINE MATMPY(M,N,H,G,S)
DIMENSION H(20,20),G(20),S(20)

700 DO 720 II=1, M
S(II)=0.0
DO 720 JJ=1,N

720 S(II)=H(JJ,II)*G(JJ)+S(II)

740 RETURN
END

```
SUBROUTINE A 14
    COMMON /400/ H(20,20), Y(20), G(20), S(20), XP(20), GP(20), T(20),
      GB(20), F, GS, EL, SL, FP, GSP, TO, Z, 7, 4, GSS, FO, GTP, FP, GTI, GSB,
   2 DELTA, E, N, MS, IT, L, IHOLD (20), NSSA1, NSSH2
300 L=1
    Z=3.0/EL+(F-FP)+35+GSP
    Q=ABS (Z+SQRT (1.0-(GS/Z)+(GSP/7)))
    A= (0-Z+GSP) / (0+0-35+GSP)
    TO=EL/3.0* (0+0+7+357) *A*A
    FO=FF-TO
    CALL MATMPY (N,N, H, GP, T)
    DO 305 I=1, N
305 T(I) = (GSP/SL) *S(I) - T(I)
    CALL MATMPY (1, N, T, GP, GTP)
    IF (TO+TO+GTF) 315,310,310
310 DO 312 I=1, N
312 T(I) = XP(I) + A^*(X(I) - XP(I))
    GO TO 340
315 IF (F+F+GTP) 310,320,320
320 DO 322 I=1, N
322 T(I) = T(I) + XP(I)
    CALL FCN(N,G3,FB,T,2)
    IF (FO-F9) 310,325,325
325 L=3
    IF (NSSW1) 100,101,100
100 WRITE(6,1)
101 DO 327 I=1,N
327 S(I) = T(I) - XP(I)
    CALL MATMPY (1,N,S,GB,GTT)
    GTT=GTT-GTP
    IF (GTT) 340,330,330
330 L=2
    GSS=CTT
    SL=-GTP
    EL=1.0
340 RETURN
  1 FORMAT (9HORICOCHET)
    END
```

```
SUBROUTINE FIRE
     COMMON /400/ H(20,20), X(20), G(20), S(20), X^2(20), GP(20), T(20),
       GB(20), F, GS, EL, SL, FP, GSP, TO, Z, J, 4, GSS, FO, GTP, FB, GTT, GSB,
       DELTA, E, N, MS, IT, L, IHOLD (20), NSS41, NSSW2
     EQUIVALENCE (TEMP, GTT)
 400 L=1
     TEMP=A/(1.0-A)
     CALL FCN(N,GB,FR,T,2)
     CALL MATMPY (1,N,S,G3,GSR)
     TO=F
     IF (TO-FP) 403, 403, 402
402 TO=FF
403 IF (TO-F8+E) 415, 405, 405
405 GSS=0+0
     TO=GSB+ (TEMP -1.0/TEMP)
     IF (ABS (T0) -0) 430,410,410
410 L=2
     GO TO 440
415
     L=3
     IF(FP-F) 425,420,420
 420 IF (NSSW1) 100, 101, 100
 100 WRITE (6,1)
 101 EL=(1.0-A)*EL
     FP=FB
     GSP=GSB
     DO 422 I=1, N
     XP(I)=T(I)
     GP(I)=GB(I)
 422 CONTINUE
     GO TC 440
 425 IF (NSSW1) 200, 201, 200
 200 WRITE (6,2)
 201 EL=EL*A
     F=FB
     GS=GSB
     00 427 I=1,N
     X(I) = T(I)
     G(I) = GP(I)
 427 CONTINUE
     GO TC 440
 430 GSS=GSS+T0
     DO 435 I=1,N
 475 G(I) = (GB(I) -G(I)) + TEMP+(GP(I) -G3(I)) / TEMP
 440 RETURN
   1 FORMAT (10HOMOVE LEFT)
   2 FORMAT (11HOMOVE RIGHT)
     END
```

```
SUBROUTINE DRESS
    COMMON /A00/ H(20, 20), Y(20), G(20), S(20), XP(20), GP(20), T(20),
      GB(20), F, G3, EL, SL, FP, GSP, T0, 7, 7, A, 3SS, F0, GTP, F8, GTT, GSB,
      DELTA, E, N, MS, II, L, IHOLD (20), NSSA1, NSSW2
500 GO TO (505, 520, 530, 325), L
505 CALL MATMPY (N,N,H,G,X)
    CALL MATMPY (1,N, X, G, TO)
    IF (TO-GSS**2/SL-5) 515,510,510
510 NO 512 II=1.N
    DO 512 JJ=1,N
512 H(II,JJ)=H(II,JJ)-X(II)*X(JJ)/T0
    DELTA=DELTA*(EL*3SS/TO)
    TO=EL/GSS
    GO TO 525
515 IF (NSSW1) 200,520,200
200 WRITF(6,1)
520 DELTA=DELTA* (EL*SL/GSS)
    TO=EL/GSS-1.0/SL
525 DO 527 II=1,N
    DO 527 JJ=1,N
(LU) 2*(II) 2*0T+(LU, II) H=(LU, II) H 75 €
530 IT=IT+1
    F=FB
    IF (NSSW1) 130, 101, 100
100 WRITE(6,4) IT,MS,F,GS
101 DO 532 I=1, N
    G(I) = GB(I)
    X(I) = T(I)
532 CONTINUE
    IF (NSSW1) 535, 540, 535
575 WRITE(6,2) (X(I),I=1,N)
    WRITF(6,3) DELTA
540 RETURN
  1 FORMAT (9HOCOLINEST)
  2 FORMAT (3HOX=,8E14.5/(3HO ,8E14.5))
  3 FORMAT (7HODELTA=, £14.5/20H0- - -
  4 FORMAT(4HOIT ,14,7H STEP ,14,4H F=, E14.5,5H GS=,E14.5)
    END
    SUBROUTINE ORDER
    COMMON /401/ HH(20,20), PER(20), GR(21), S(20), XP(20), GP(20), T(20),
       GB(20), F, GS, EL, SL, FP, GSP, TO, Z, J, A, GSS, FO, GTP, FB, GTT, GSB,
      DELTA, E, N, MS, IT, L, IHOLD (20), NSS 41, NSSW2
    JC = N - 1
    DO 100 I=1,JC
    K = I + 1
    DO 100 J=K.N
    IF (PER(I)-PER(J)) 100,100,60
 50 SAVE = PER(I)
    PER(I) = PER(J)
    PER(J) = SAVE
    SAVE = HH(I, I)
    (L,L)HH = (I,I)HH
    HH (J, J) = SAVE
    ISAV = IHOLD(I)
    IHOLD(I) = IHOLD(J)
    IHOLD(J) = ISAV
170 CONTINUE
    RETURN
    END
                                  117
```

Appendix I

Miscellaneous Plots

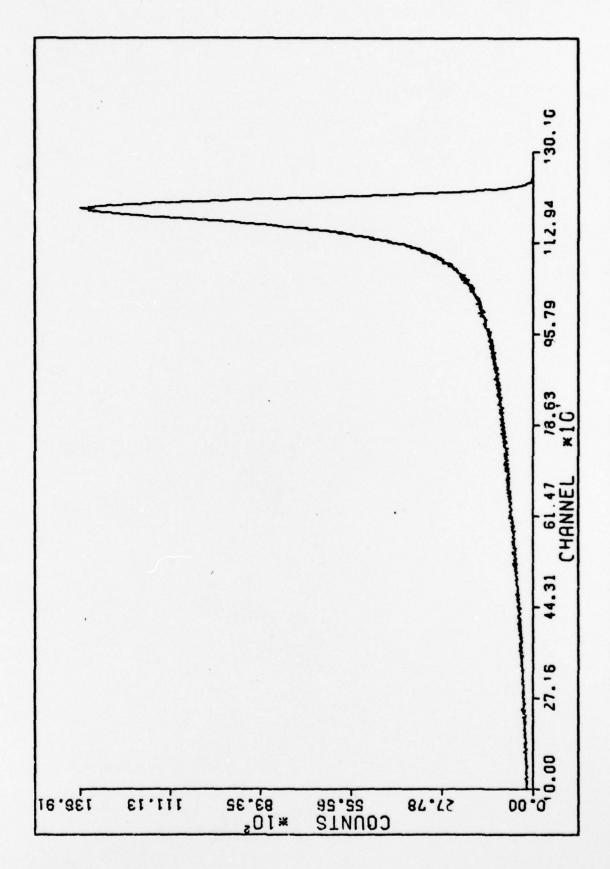


FIG 25. RR DEF # 11 (UNDX101ZED) 0.6 KEV/CHANNEL 40.000 SEC.

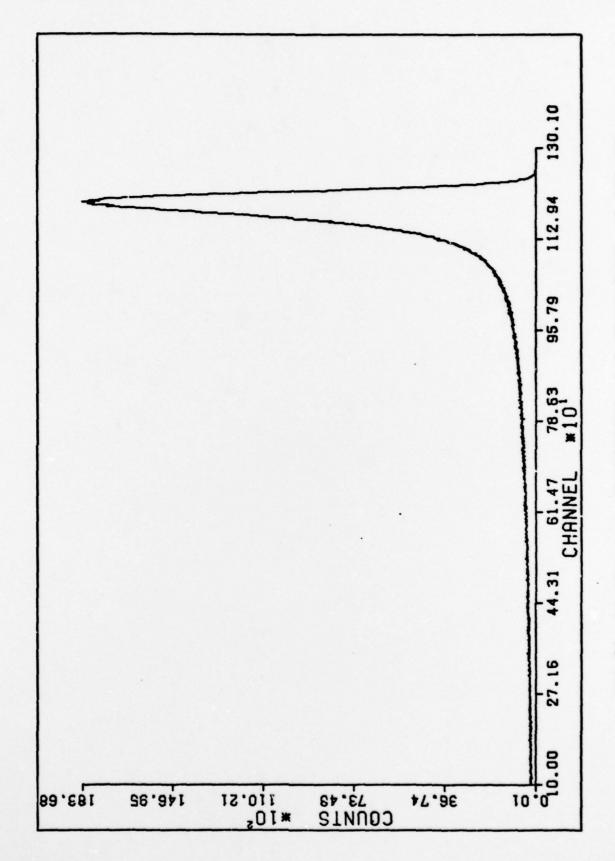


FIG 26. RR DEF # 12 (UNDXIDIZED) D.6 KEV/CHANNEL 40.000 SEC.

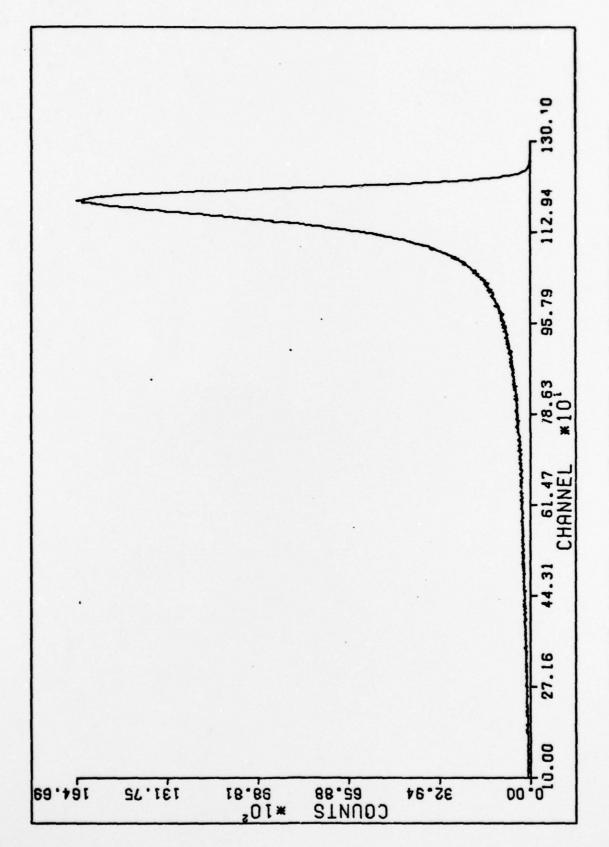


FIG 27. RR DEF # 13 (UNBXIDIZED) 0.6 KEV/CHRNNEL 40.000 SEC.

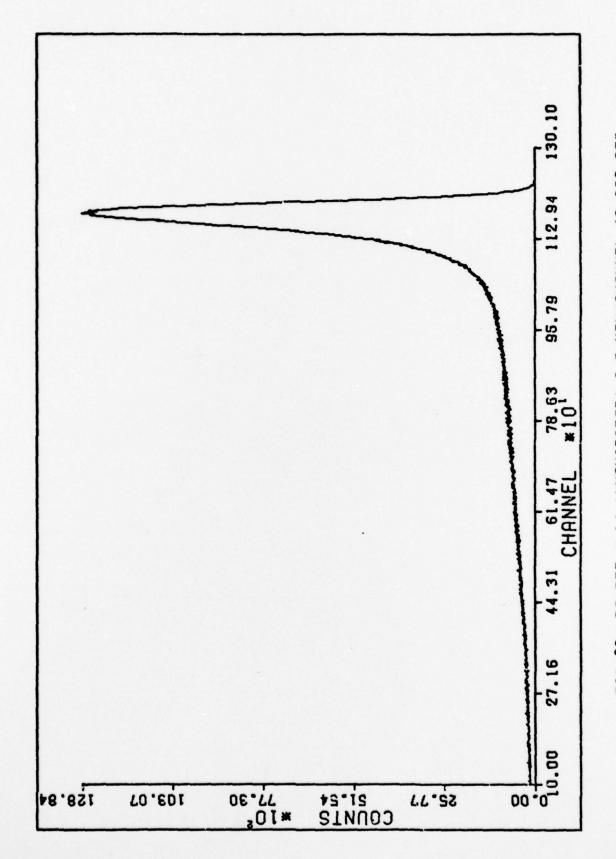


FIG 28. RR DEF # 14 (UNBXIDIZED) 0.6 KEV/CHRNNEL 40.000 SEC.

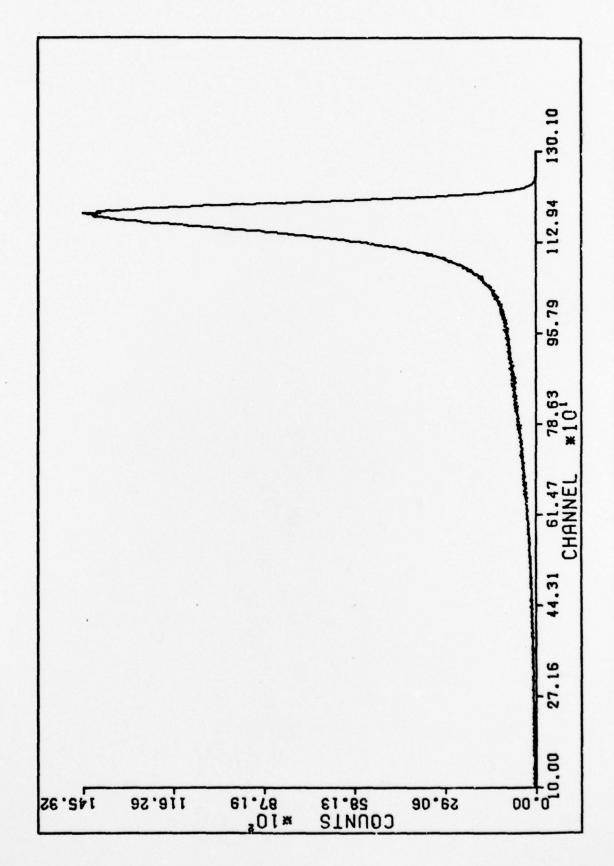


FIG 29 RA DEF # 15 (UNOXIDIZED) 0.6 KEV/CHANNEL 40000 SEC.

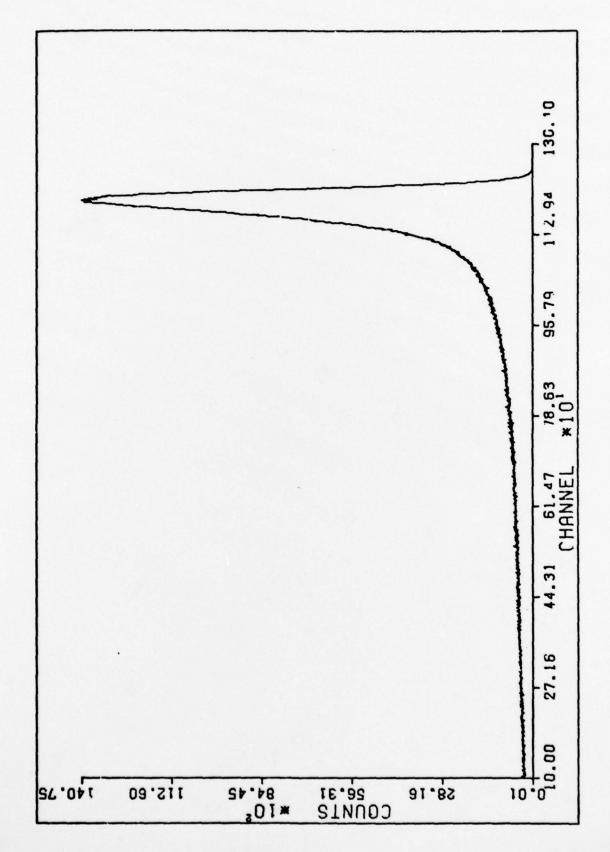


FIG 30. RR DEF # 16 (UNOXIDIZED) 0.6 KEV/CHRNNEL 40.000 SEC.

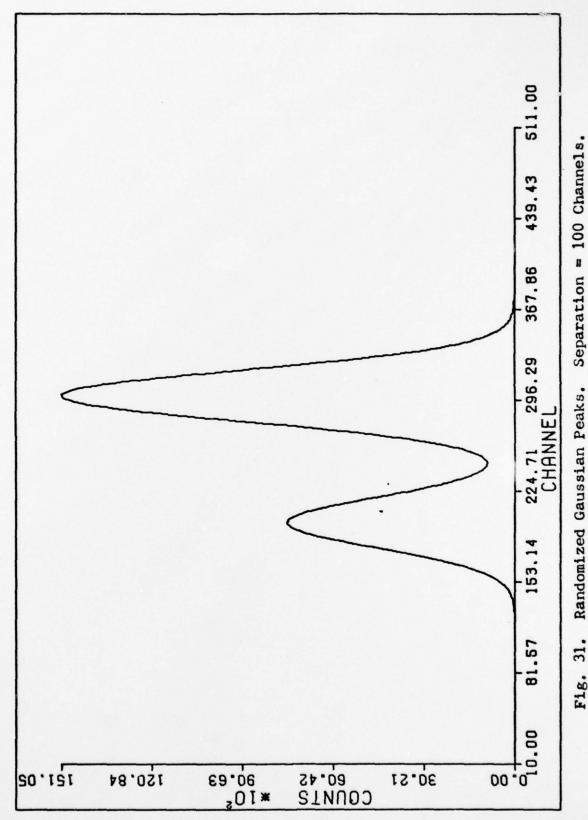
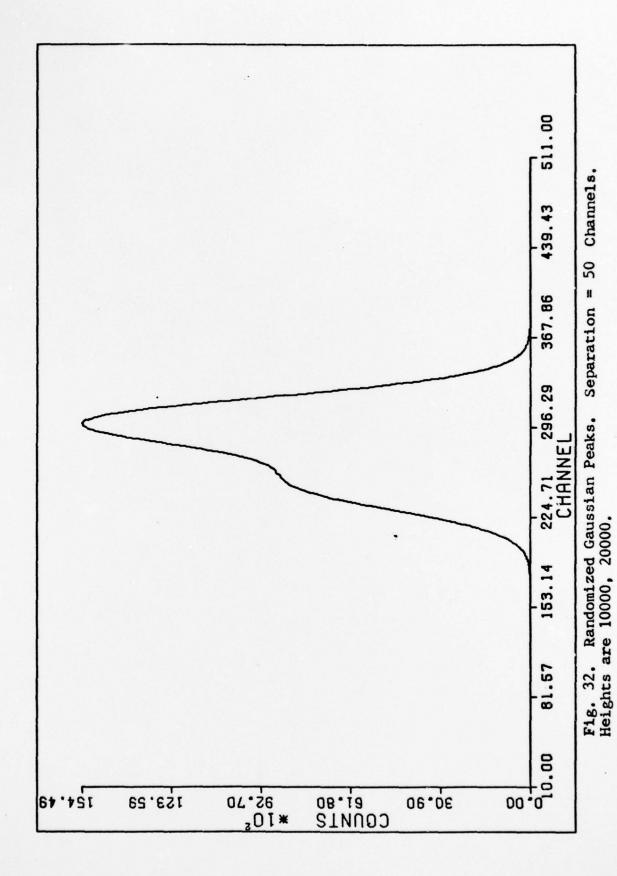


Fig. 31. Randomized Gaussian Peaks. Heights are 10000, 20000.



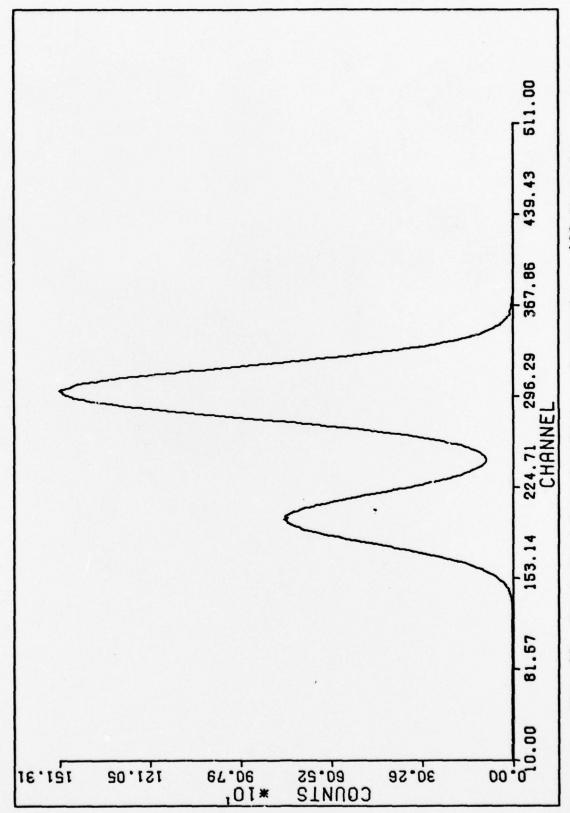
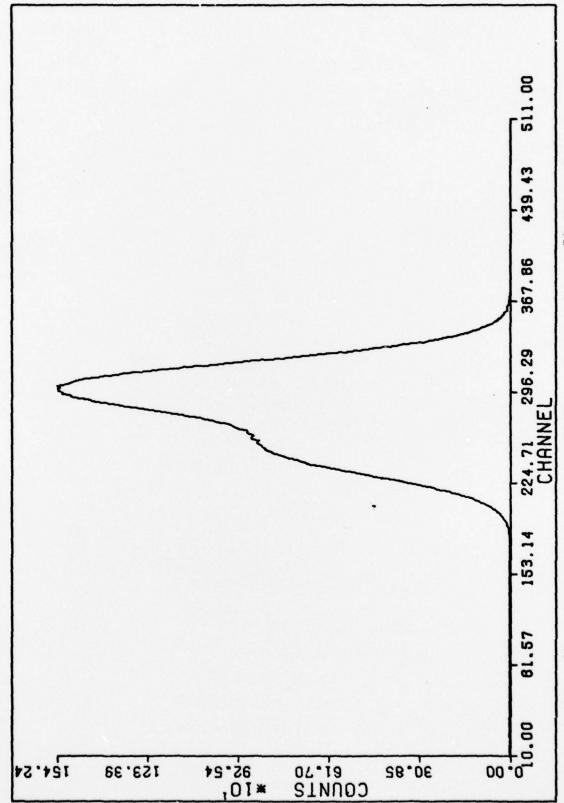
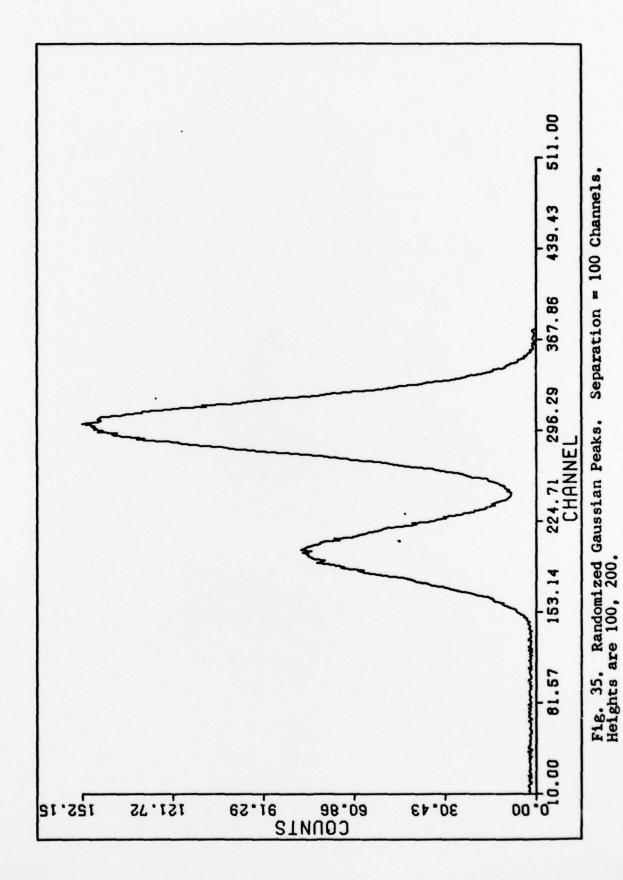


Fig. 33. Randomized Gaussian Peaks. Separation = 100 Channels. Heights are 1000, 2000.



Separation = 50 Channels. Fig. 34. Randomized Gaussian Peaks. Heights are 1000, 2000.



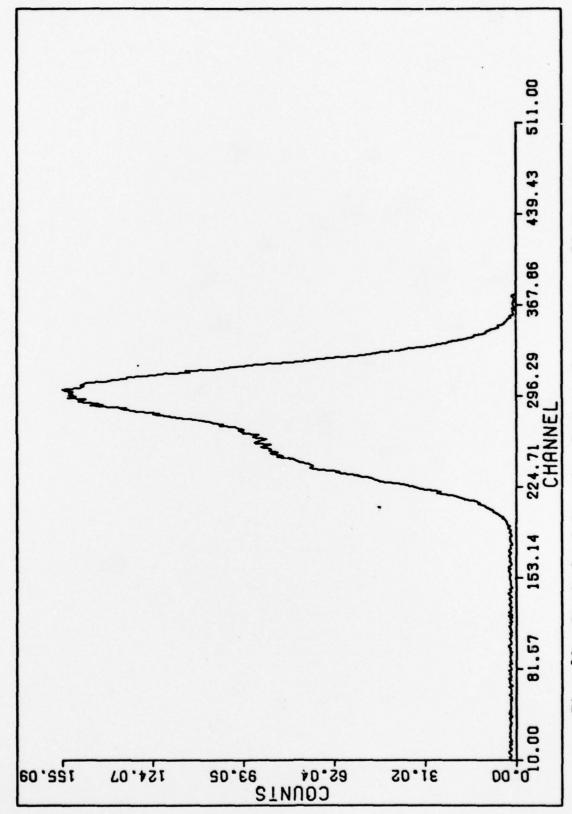


Fig. 36. Randomized Gaussian Peaks. Separation = 50 Channels. Heights are 100, 200.

Vita

John Robert Harstine was born on 14 February 1950 in Tulsa, Oklahoma. He graduated from El Dorado High School in El Dorado, Kansas, in 1968 and attended the Lyman Briggs College of Michigan State University from which he received the degree of Bachelor of Science in Physics in 1972. He received a commission in the United States Air Force through the ROTC program and began active duty in November of 1972. After receiving technical training at Sheppard Air Force Base, Texas, and Vandenberg Air Force Base, California, he served as a missile launch officer in the Titan II ICBM at Davis-Monthan Air Force Base, Arizona. He entered the School of Engineering, Air Force Institute of Technology, in August of 1977.

Permanent address: 1911 Arlington
El Dorado, Kansas 67042

SECURITY CLASSIFICATION OF THIS PAGE (When Date Entered)

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
AFIT/GNE/PH/78D-/6	3. RECIPIENT'S CAYALOG NUMBER
4. TITLE (and Subtitle) COMPUTER CODE TO ANALYZE ALPHA SPECTRA	5. TYPE OF REPORT & PERIOD COVERED MS Thesis
USING A SPECTRAL STRIPPING APPROACH	6. PERFORMING ORG. REPORT NUMBER
John R. Harstine Captain USAF	8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT PROJECT TASK
Air Force Institute of Technology(AFIT-EN) Wright-Patterson AFB, Ohio 45433	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE
McClellan Central Laboratory 1155th Technical Operation Squadron McClellan AFB, CA 95652	December 1978 13. NUMBER OF PAGES 142
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report)
	Unclassified
	15m. DECLASSIFICATION DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report)	
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)	
16. SUPPLEMENTARY NOTES	
Approved for public release; IAW AFR 190-17	
Joseph P. Hipps Major, USAF Director of Information 19. Kerwords (Continue on reverse side if necessary and identity by block number)	
Alpha Spectrometry	
Americium Plutonium	
Polonium	
Surface Barrier Detectors 20. ABSTRACT (Continue on reverse side of necessary and identity by block number)	
Sources of Po of varying thicknesses were prepared by an evaporative precipitation method. Sources of Am240 and Pu240 were analyzed with the spectra of these sources as reference peak	
functions using a modification of an existing computer code. The results showed a reduction of the residual from using a reference peak with a full width at half maximum close to that of the	
analyzed source. The performance of the computer code was also studied using randomized Gaussian peaks.	

DD 1 1473 EDITION OF 1 NOV 65 IS OBSOLETE

SECURITY CLASSIFICATION OF THIS PAGE (When Date Entered)